

Access DB# 162740**SEARCH REQUEST FORM****Scientific and Technical Information Center**

Requester's Full Name: Dr. A. D. W. Examiner #: 69332 Date: 8/16/85
 Art Unit: 1711 Phone Number 30 2-881 Serial Number: 6/661,812
 Mail Box and Bldg/Room Location: 6D71 Results Format Preferred (circle): PAPER DISK E-MAIL

If more than one search is submitted, please prioritize searches in order of need.

Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc, if known. Please attach a copy of the cover sheet, pertinent claims, and abstract.

Title of Invention: _____

Inventors (please provide full names): _____

SCIENTIFIC REFERENCE BR
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Earliest Priority Filing Date: _____

**For Sequence Searches Only* Please include all pertinent information (parent, child, divisional, or issued parent numbers) along with the appropriate serial number.*

Pat. & T.M. Office

Formula Ia in claim 14. in that R₁ and R₂ has been defined in claim 1.
 Thanks.

STAFF USE ONLY

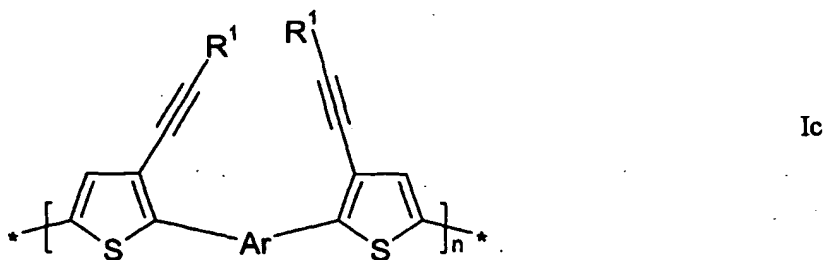
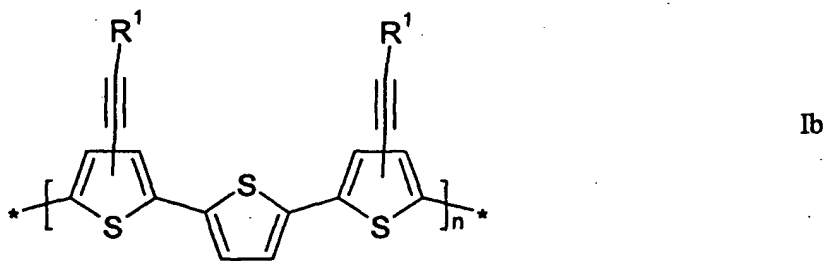
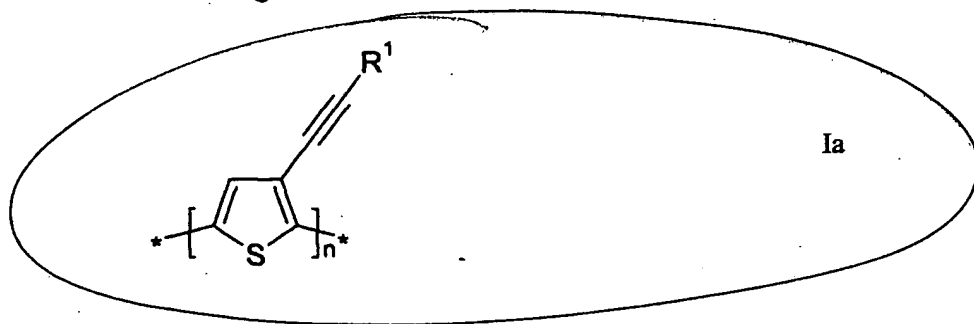
	Type of Search	Vendors and cost where applicable
Searcher: <u>ES</u>	NA Sequence (#) _____	STN _____
Searcher Phone #: _____	AA Sequence (#) _____	Dialog _____
Searcher Location: _____	Structure (#) _____	Questel/Orbit _____
Date Searcher Picked Up: _____	Bibliographic _____	Dr.Link _____
Date Completed: <u>9-1-05</u>	Litigation _____	Lexis/Nexis _____
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Clerical Prep Time: _____	Patent Family _____	WWW/Internet _____
Online Time: _____	Other _____	Other (specify) _____

h/ 661,812

- 40 -

(O)_{k2}-, Phe-CH=CH-, HOOC-, OCN-, and W⁴W⁵W⁶Si-, with W¹ being H, Cl, CN, phenyl or alkyl with 1 to 5 C-atoms, W² and W³ being independently of each other H or alkyl with 1 to 5 C-atoms, W⁴, W⁵ and W⁶ being independently of each other Cl, oxaalkyl or oxacarbonylalkyl with 1 to 5 C-atoms, Phe being 1,4-phenylene and k₁ and k₂ being independently of each other 0 or 1.

14. A monomer, oligomer or polymer according to claim 1, wherein -[(A)_a-(B)_b-(C)_c-(D)_d] is selected from the following formulae



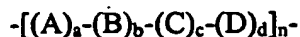
6/661,812

1-15

- 36 -

CLAIMS

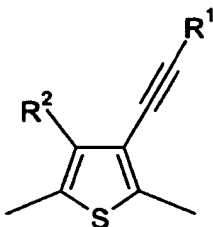
1. A monomer, oligomer or polymer of formula I



I

wherein

A and C denote independently of each other a group of formula II



II

R^1 is in each occurrence independently of one another H, halogen, or straight chain, branched or cyclic alkyl with 1 to 20 C-atoms, which is unsubstituted, mono- or poly-substituted by F, Cl, Br, I or CN, wherein one or more non-adjacent CH_2 groups are optionally replaced, in each case independently from one another, by $-O-$, $-S-$, $-NH-$, $-NR^0-$, $-SiR^0R^{00}-$, $-CO-$, $-COO-$, $-OCO-$, $-OCO-O-$, $-SO_2-$, $-S-CO-$, $-CO-S-$, $-CH=CH-$ or $-C\equiv C-$ in such a manner that O and/or S atoms are not linked directly to one another, or R^1 denotes optionally substituted aryl or heteroaryl or P-Sp-,

R^2 has one of the meanings of R^1 or denotes $-C\equiv C-R^3$,

R^3 has one of the meanings of R^1 ,

R^0 and R^{00} are independently of each other H or alkyl with 1 to 12 C-atoms,

P is a polymerizable or reactive group,

Sp is a spacer group or a single bond,

$n \geq 1$

=> file reg

FILE 'REGISTRY' ENTERED AT 11:26:00 ON 01 SEP 2005
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L1 FILE 'LREGISTRY' ENTERED AT 10:48:50 ON 01 SEP 2005
STR

L2 FILE 'REGISTRY' ENTERED AT 10:50:00 ON 01 SEP 2005
SCR 2043
L3 2 S L1 AND L2

L4 FILE 'HCAPLUS' ENTERED AT 10:54:19 ON 01 SEP 2005
209 S HEENEY ?/AU
L5 900 S TIERNEY ?/AU
L6 16746 S BAILEY ?/AU
L7 17 S L4 AND L5 AND L6
L8 52 S HEENEY M?/AU
L9 49 S TIERNEY S?/AU
L10 1212 S BAILEY C?/AU
L11 17 S L8 AND L9 AND L10
SEL L11 10 RN

L12 FILE 'REGISTRY' ENTERED AT 10:56:40 ON 01 SEP 2005
1 S E1

L13 FILE 'HCA' ENTERED AT 10:57:22 ON 01 SEP 2005
34 S L12
E ELECTRIC CONDUCTORS/CV
L14 60618 S E3
L15 95308 S (ELECTROLUM!N? OR ORGANOLUM!N? OR (ELECTRO OR ORGANO OR
E ANISOTROPIC MATERIALS/CV
L16 622 S E3
L17 18452 S (PHOSPHORES? OR PHOSPHOR# OR LUMINES? OR FLUORES?) (2A) (
L18 22333 S ANTISTATIC?
E OPTICAL IMAGING DEVICES/CV
L19 33625 S E3
L20 87325 S (CHARG? OR HOLE# OR ELECTRON# OR E) (2A) (TRANSPORT? OR I
L21 65225 S ELECTROPHOTOG?
L22 37301 S FET OR FIELD? (3A) EFFECT? (3A) TRANSISTOR?
E LIQUID CRYSTALS/CV
L23 75951 S E3

L24 24397 E LIQUID CRYSTAL DISPLAYS/CV
 S E3
 E PHOTOCONDUCTORS/CV
 L25 3811 S E3
 L26 70151 S PHOTOELECTRIC? OR PHOTO(A) (ELEC# OR ELECTRIC?)
 E SAFETY DEVICES/CV
 L27 4512 S E3
 E SENSORS/CV
 L28 28473 S E3
 L29 17051 S TFT OR (THINFILM? OR THIN? (A) FILM?) (3A) TRANSISTOR?
 E CONDUCTING POLYMERS/CV
 L30 10788 S E3
 L31 2 S L13 AND (L14-L30)

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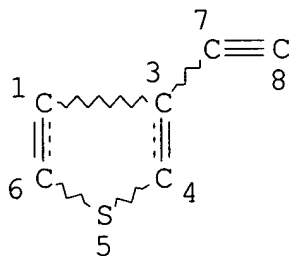
L32 33 S L1
 L33 STR L1
 L34 27 S L33
 L35 656 S L33 FUL
 SAV L35 TRU812/A
 L36 24 S L35 AND PMS/CI

FILE 'HCA' ENTERED AT 11:23:13 ON 01 SEP 2005

L37 26 S L36
 L38 287 S L35
 L39 26 S L38 AND (L14-L30)
 L40 18 S (L31 OR L39) NOT L37
 L41 30 S L13 NOT (L37 OR L40)

FILE 'REGISTRY' ENTERED AT 11:26:00 ON 01 SEP 2005

=> d l35 que stat
 L33 STR



NODE ATTRIBUTES:
 DEFAULT MLEVEL IS ATOM
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RSPEC I

NUMBER OF NODES IS 7

STEREO ATTRIBUTES: NONE

L35 656 SEA FILE=REGISTRY SSS FUL L33

100.0% PROCESSED 3541 ITERATIONS

656 ANSWERS

SEARCH TIME: 00.00.01

=> file hca

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=> d l37 1-26 cbib abs hitstr hitrn

L37 ANSWER 1 OF 26 HCA COPYRIGHT 2005 ACS on STN

142:7139 Stability of substituted poly(acetylene)s. Law, Charles C. W.; Lam, Jacky W. Y.; Dong, Yuping; Tang, Ben Zhong (Department of Chemistry, The Hong Kong University of Science and Technology, Kowloon, Hong Kong). Polymer Preprints (American Chemical Society, Division of Polymer Chemistry), 45(2), 829-830 (English) 2004. CODEN: ACPPAY. ISSN: 0032-3934. Publisher: American Chemical Society, Division of Polymer Chemistry.

AB Stability of substituted polyacetylenes in air is studied. Poly(arylacetylene) such as poly(phenylacetylene) is thermally unstable in air, degrading into oligomers at high temps. The stability is still low when it is substituted. For poly(1-alkyne) system, the incorporation of arom. pendent groups into the polymer structures has endowed the polymers with high thermal stability, which experience little mol. wt. change even when heated to 200.degree. in air. The polymers are also stable in soln. and resistant to UV irradiation in air. The disubstituted polyacetylenes show superior thermal stability and no mol. wt. drop is obsd. even when the polymers are annealed at 200.degree. in air for 12 h.

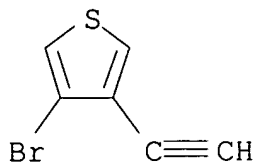
IT **225244-01-9**
(thermal stability of substituted polyacetylenes)

RN 225244-01-9 HCA

CN Thiophene, 3-bromo-4-ethynyl-, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 198491-48-4
CMF C6 H3 Br S



IT **225244-01-9**
(thermal stability of substituted polyacetylenes)

L37 ANSWER 2 OF 26 HCA COPYRIGHT 2005 ACS on STN
141:317214 Fullerene-containing conducting polymers with good mechanical properties and light resistance, their manufacture, and organic solar cells. Murata, Seijiro; Komatsu, Koichi; Yamazaki, Tetsuya; Fujita, Shizuo (Kyoto University, Japan; Nippon Telegraph and Telephone Corp.; Pioneer Electronic Corp.; Hitachi Ltd.; Mitsubishi Chemical Corp.; Rohm Co., Ltd.). Jpn. Kokai Tokkyo Koho JP 2004277736 A2 20041007, 28 pp. (Japanese). CODEN: JKXXAF. APPLICATION: JP 2004-55245 20040227. PRIORITY: JP 2003-54336 20030228.

AB The polymers comprise connected thiophene rings having CN- or Me-contg. fullerene groups in side chains. The polymers may be manufd. by coupling reaction of thiophene derivs. and 2,3,5-tribromothiophene for manuf. of bromoterthiophene derivs., coupling reaction of the bromoterthiophene derivs. with trimethylsilylacetylene for manuf. of acetylene derivs., lithiation of the acetylene derivs. with tetrabutylammonium fluoride and BuLi, dissolving the lithiated derivs. in fullerene-contg. o-dichlorobenzene for manuf. of fullerene anions, reaction of the fullerene anions with tosyl cyanide or Me group for manuf. of terthiophene-fullerene monomers, and polymn. of the monomers. The polymers show improved electrocond. and charge sepn. property, and are useful for org. solar cells with high photoelec. conversion efficiency.

IT **665003-44-1P 765900-27-4P**
(manuf. of fullerene-contg. conducting polythiophenes with good mech. properties and light resistance for org. solar cells)

RN 665003-44-1 HCA
CN Thieno[3,4-b]-1,4-dioxin, 5,5'-[3-[(9-methyl[5,6]fulleren-C60-Ih-1(9H)-yl)ethynyl]-2,5-thiophenediyl]bis[2,3-dihydro-, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 665003-42-9

CMF C79 H14 O4 S3

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

RN 765900-27-4 HCA

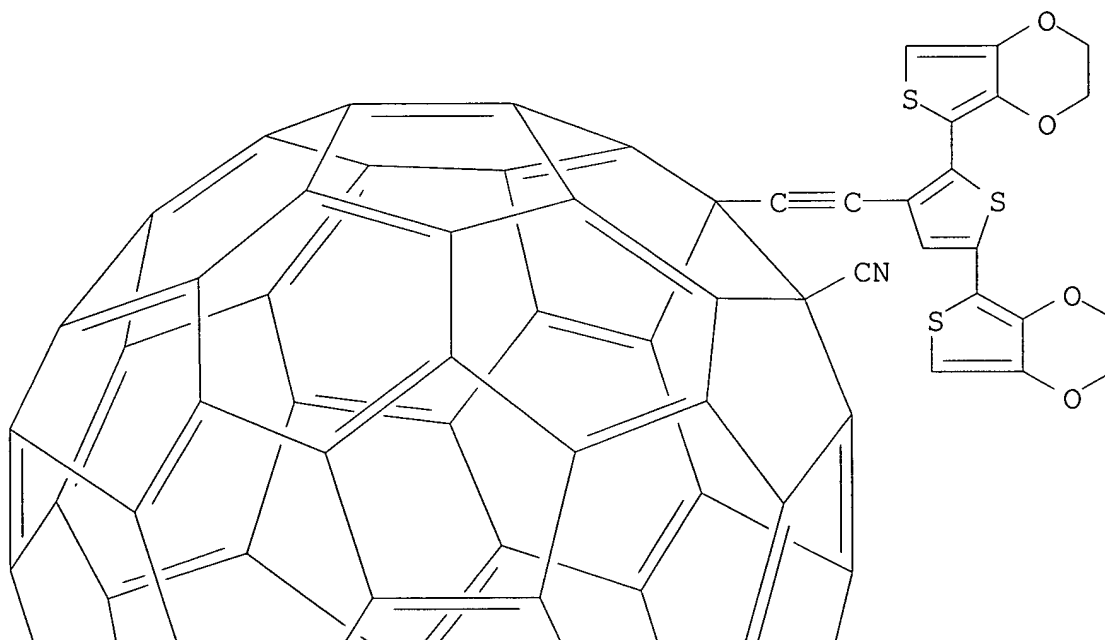
CN [5,6]Fullerene-C60-Ih-1(9H)-carbonitrile, 9-[[2,5-bis(2,3-dihydrothieno[3,4-b]-1,4-dioxin-5-yl)-3-thienyl]ethynyl]-, homopolymer (9CI) (CA INDEX NAME)

CM 1

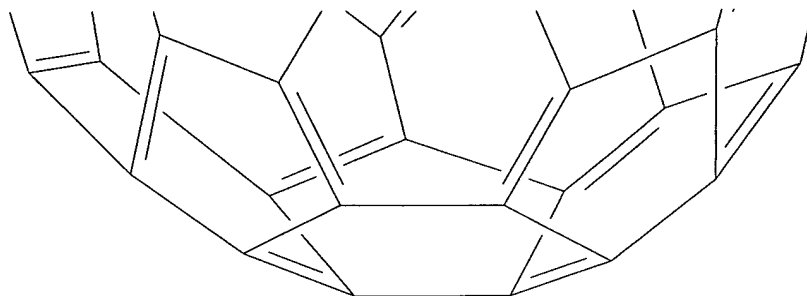
CRN 765900-24-1

CMF C79 H11 N O4 S3

PAGE 1-A



PAGE 2-A



IT **665003-44-1P 765900-27-4P**

(manuf. of fullerene-contg. conducting polythiophenes with good mech. properties and light resistance for org. solar cells)

L37 ANSWER 3 OF 26 HCA COPYRIGHT 2005 ACS on STN

140:218181 Synthesis and electrolytic polymerization of fullerene-terthiophene dyads. Murata, Yasujiro; Suzuki, Mitsuharu; Yamazaki, Tetsuya; Komatsu, Koichi (Institute for Chemical Research, Kyoto University, Kyoto, 611-0011, Japan). Proceedings - Electrochemical Society, 2003-15(Fullerenes--Volume 13: Fullerenes and Nanotubes), 316-322 (English) 2003. CODEN: PESODO. ISSN: 0161-6374. Publisher: Electrochemical Society.

AB Novel fullerene derivs. having a terthiophene moiety connected by a triple bond were synthesized by nucleophilic addn. of the lithium acetylides connected to terthiophene to C60. Electropolymn. of these dyads afforded the electroactive polymer films which were stable both in p-doped and n-doped states.

IT **630402-67-4P 665003-44-1P**

(synthesis and electrolytic polymn. of fullerene-terthiophene dyads)

RN 630402-67-4 HCA

CN 2,2':5',2''-Terthiophene, 3'-[(9-methyl[5,6]fulleren-C60-Ih-1(9H)-yl)ethynyl]-, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 630402-65-2

CMF C75 H10 S3

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

RN 665003-44-1 HCA

CN Thieno[3,4-b]-1,4-dioxin, 5,5'-[3-[(9-methyl[5,6]fulleren-C60-Ih-1(9H)-yl)ethynyl]-2,5-thiophenediyl]bis[2,3-dihydro-, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 665003-42-9
CMF C79 H14 O4 S3

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

IT **630402-67-4P 630402-67-4P 665003-44-1P**
665003-44-1P

(synthesis and electrolytic polymn. of fullerene-terthiophene dyads)

L37 ANSWER 4 OF 26 HCA COPYRIGHT 2005 ACS on STN

140:17072 Synthesis and electropolymerization of fullerene-terthiophene dyads. Murata, Yasujiro; Suzuki, Mitsuharu; Komatsu, Koichi (Institute for Chemical Research, Kyoto University, Uji, Japan). Organic & Biomolecular Chemistry, 1(15), 2624-2625 (English) 2003. CODEN: OBCRAK. ISSN: 1477-0520. Publisher: Royal Society of Chemistry.

AB Fullerene derivs. having a terthiophene unit connected by a triple bond were synthesized and electroactive polymers were obtained by electrolytic oxidn. of the terthiophene moiety.

IT **630402-66-3P 630402-67-4P**
(synthesis and electropolymn. of fullerene-terthiophene dyads)

RN 630402-66-3 HCA

CN 2,2':5',2''-Terthiophene, 3'-([5,6]fulleren-C60-Ih-1(9H)-ylethynyl)-, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 630402-64-1
CMF C74 H8 S3

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

RN 630402-67-4 HCA

CN 2,2':5',2''-Terthiophene, 3'-[(9-methyl[5,6]fulleren-C60-Ih-1(9H)-yl)ethynyl]-, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 630402-65-2
CMF C75 H10 S3

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

IT **630402-66-3P 630402-67-4P**

(synthesis and electropolymn. of fullerene-terthiophene dyads)

L37 ANSWER 5 OF 26 HCA COPYRIGHT 2005 ACS on STN

140:5359 Photo-induced cis-to-trans isomerization monosubstituted polyacetylenes bearing a thiophene ring prepared with a Rh complex catalyst. Tabata, Masayoshi; Miyasaka, Atsushi; Nakamura, Minoru; Mawatari, Yasuteru (Department of Molecular Chemistry, Graduate School of Engineering, Hokkaido University, Sapporo, 060-8628,

Japan). Polymer Preprints (American Chemical Society, Division of Polymer Chemistry), 44(2), 819-820 (English) 2003. CODEN: ACPPAY. ISSN: 0032-3934. Publisher: American Chemical Society, Division of Polymer Chemistry.

AB Ethynylthiophenes were successfully polymd. using a [Rh(norbornadiene)Cl]₂ catalyst in the presence of triethylamine or ethanol as the polymn. solvent to produce the poly(2-ethynylthiophene), P2ET, polymers. The resulting polyacetylenes were characterized in detailed using H NMR, soln. and film UV-Vis, and ESR methods. The difference in the color of their polymers prepd. using TEA or EtOH solvent was suggested in terms of the difference in the degree of the aggregation of the polymer chains. Photoinduced cis-to-trans isomerization of the pristine polymer was newly found to occur when the polymer was irradiated using light of 320-470 nm under vacuum for 5 h. The obtained trans isomer was also studied in detail using ESR and UV- Vis spectra. The data showed that the distorted trans conjugation sequences were formed in the solid phase where a large no. of radicals produced by the rotational scission of the cis C=C bonds is stabilized.

IT **97418-70-7P**, Poly(3-ethynylthiophene)
(photo-induced cis-to-trans isomerization monosubstituted polyacetylenes bearing a thiophene ring prepd. with a Rh complex catalyst)

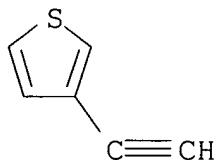
RN 97418-70-7 HCA

CN Thiophene, 3-ethynyl-, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 67237-53-0

CMF C6 H4 S



IT **97418-70-7P**, Poly(3-ethynylthiophene)
(photo-induced cis-to-trans isomerization monosubstituted polyacetylenes bearing a thiophene ring prepd. with a Rh complex catalyst)

L37 ANSWER 6 OF 26 HCA COPYRIGHT 2005 ACS on STN

137:279554 Synthesis and properties of coil-shaped 2,3-thienylene-ethynylene oligomers. Aso, Yoshio; Obara, Yuko; Okai, Takashi; Nishiguchi, Shoji; Otsubo, Tetsuo (Faculty of Engineering, Hiroshima University, Higashi-Hiroshima, 739-8527, Japan). Molecular Crystals

and Liquid Crystals Science and Technology, Section A: Molecular Crystals and Liquid Crystals, 376, 153-158 (English) 2002. CODEN: MCLCE9. ISSN: 1058-725X. Publisher: Taylor & Francis Ltd..

AB A series of 2,3-thienylene-ethynylene oligomers have been synthesized by repeated application of the Pd-catalyzed coupling reaction of terminal alkyne and thienyl iodides as the key building steps. The anal. GPC mol. wts., much deflated relative to the actual mol. wts., strongly suggest a coil shape for the conformation of the oligomers in soln. Their electronic absorption and emission spectral features are discussed.

IT **467251-61-2P 467251-62-3P**

(Pd-catalyzed coupling synthesis and soln. coil chain conformation of 2,3-thienylene-ethynylene oligomers)

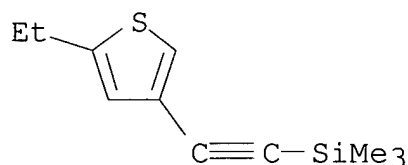
RN 467251-61-2 HCA

CN Silane, [(5-ethyl-3-thienyl)ethynyl]trimethyl-, homopolymer (9CI)
(CA INDEX NAME)

CM 1

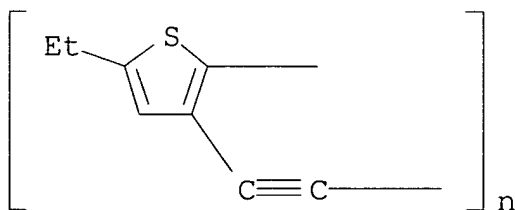
CRN 467251-52-1

CMF C11 H16 S Si



RN 467251-62-3 HCA

CN Poly[(5-ethyl-2,3-thiophenediyl)-1,2-ethynediyl] (9CI) (CA INDEX NAME)



IT **467251-61-2DP**, desilylated

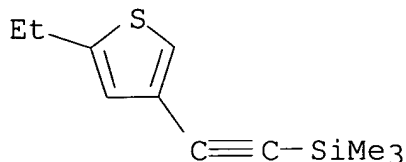
(Pd-catalyzed coupling synthesis and soln. coil chain conformation of 2,3-thienylene-ethynylene oligomers)

RN 467251-61-2 HCA

CN Silane, [(5-ethyl-3-thienyl)ethynyl]trimethyl-, homopolymer (9CI)
(CA INDEX NAME)

CM 1

CRN 467251-52-1
CMF C11 H16 S Si



IT **467251-61-2P 467251-62-3P**

(Pd-catalyzed coupling synthesis and soln. coil chain conformation of 2,3-thienylene-ethynylene oligomers)

IT **467251-61-2DP, desilylated**

(Pd-catalyzed coupling synthesis and soln. coil chain conformation of 2,3-thienylene-ethynylene oligomers)

L37 ANSWER 7 OF 26 HCA COPYRIGHT 2005 ACS on STN

135:153178 Preparation and properties of polythiophene with phenylacetylene substituent. Hayashi, Hideki; Yamamoto, Takakazu (Chemical Resources Laboratory, Tokyo Institute of Technology, Nagatsuta, Midori-ku, Yokohama), 226-8503, Japan). Kobunshi Ronbunshu, 58(5), 221-226 (Japanese) 2001. CODEN: KBRBA3. ISSN: 0386-2186. Publisher: Kobunshi Gakkai.

AB Dehalogenative polycondensation of 2,5-dibromo-3-(4-alkylphenylethynyl)thiophenes with zerovalent nickel complexes afforded poly[3-(4-alkylphenylethynyl)thiophene-2,5-diyl]s in good yields. Anal., IR, and ¹³C NMR data agreed with the structure of the polymers. The UV-vis. absorption peak of the polymer appeared at a longer wavelength than the peaks of poly(3-alkylthiophene) and poly(3-arylthiophene), suggesting the formation of a larger effective .pi.-conjugation system due to negligible steric repulsion between the substituent and the neighboring thiophene unit. Cyclic voltammetry of the polymer indicated that alkylphenylethynyl substituent behaved as an electron-withdrawing unit.

IT **352711-80-9P 352711-81-0P 352711-82-1P**

352711-83-2P 352711-84-3P 352711-85-4P

(prepn. and properties of polythiophene with phenylacetylene substituent)

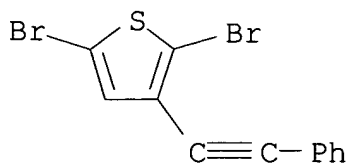
RN 352711-80-9 HCA

CN Thiophene, 2,5-dibromo-3-(phenylethynyl)-, homopolymer (9CI) (CA INDEX NAME)

CM 1

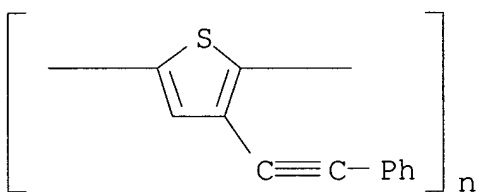
CRN 352711-77-4

CMF C12 H6 Br2 S



RN 352711-81-0 HCA

CN Poly[3-(phenylethynyl)-2,5-thiophenediyl] (9CI) (CA INDEX NAME)



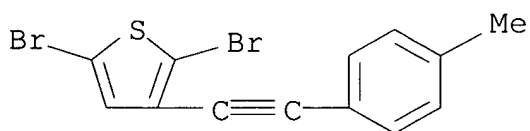
RN 352711-82-1 HCA

CN Thiophene, 2,5-dibromo-3-[(4-methylphenyl)ethynyl]-, homopolymer (9CI) (CA INDEX NAME)

CM 1

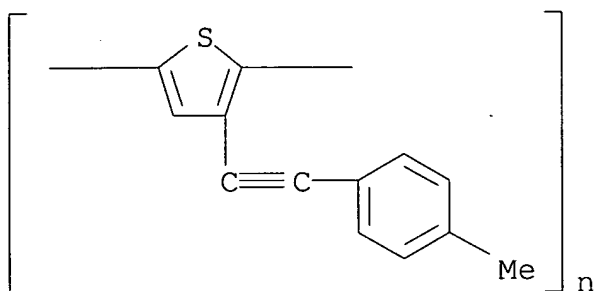
CRN 352711-78-5

CMF C13 H8 Br2 S



RN 352711-83-2 HCA

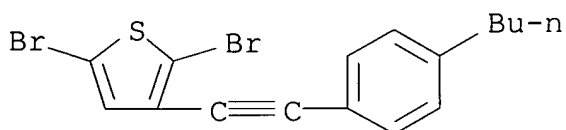
CN Poly[3-[(4-methylphenyl)ethynyl]-2,5-thiophenediyl] (9CI) (CA INDEX NAME)



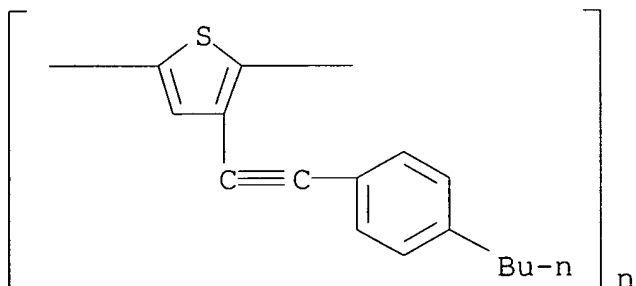
RN 352711-84-3 HCA
 CN Thiophene, 2,5-dibromo-3-[(4-butylphenyl)ethynyl]-, homopolymer
 (9CI) (CA INDEX NAME)

CM 1

CRN 352711-79-6
 CMF C16 H14 Br2 S



RN 352711-85-4 HCA
 CN Poly[3-[(4-butylphenyl)ethynyl]-2,5-thiophenediyl] (9CI) (CA INDEX NAME)

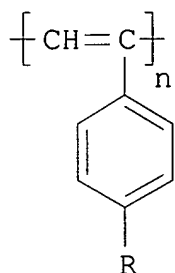


IT 352711-80-9P 352711-81-0P 352711-82-1P
 352711-83-2P 352711-84-3P 352711-85-4P
 (prepn. and properties of polythiophene with phenylacetylene
 substituent)

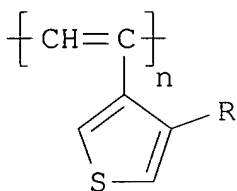
L37 ANSWER 8 OF 26 HCA COPYRIGHT 2005 ACS on STN

134:170723 Photoconductivity of substituted polyacetylenes. Chen, Hong Zheng; Xu, Rui Song; Sun, Qunhui; Lam, Jacky W. Y.; Wang, Mang; Tang, Ben Zhong (Department of Chemistry and Center for Display Research, Hong Kong University of Science and Technology, Hong Kong, Peop. Rep. China). *Polymers for Advanced Technologies*, 11(8-12), 442-449 (English) 2000. CODEN: PADTE5. ISSN: 1042-7147. Publisher: John Wiley & Sons Ltd..

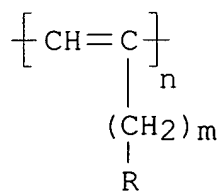
GI



I



II



III

AB Photoconduction under visible light illumination was studied using xerog. discharge technique in photoreceptors contg. p-substituted polyacetylenes I (R = H (1), Me (2), CO₂(CH₂)₆CO-p-C₆H₄-p-C₆H₄-p-OC₇H₁₅ (3)), .beta.-substituted poly(3-thienylacetylenes) II (R = SiMe₃ (4), Br (5)), and m-substituted poly(1-alkynes) III (m = 2, R = CO(CH₂)₆CO-p-C₆H₄-p-C₆H₄-p-OC₉H₁₉ (6), m = 3, R = 9-carbazolyl (7), m = 9, R = CO₂(CH₂)₆CO-p-C₆H₄-p-C₆H₄-p-OC₇H₁₅ (8)). In the undoped state, 2-4 and 6-8 showed much higher photosensitivity than (1). The polyacetylenes with electron-donating and/or hole-transporting substituents performed better than do those with electron-accepting ones. The liq. cryst. polyacetylene 6 exhibited very high photosensitivity, probably because of the cryst. aggregates of its mesogenic pendants. C60 acted as a photocond. enhancer when doped to amorphous 3 but functioned as a quencher when mixed with liq. cryst. 6. While 3 showed low photosensitivity in the undoped state, doping with I2 and sensitization with Crystal violet dramatically increased its photosensitivity up to 41.2 .times. 10⁻³ lx-1-sec-1.

IT **225244-01-9 225244-03-1**
(photocond. of substituted polyacetylene-based electrophotog. photoreceptors contg. under visible light exposure)

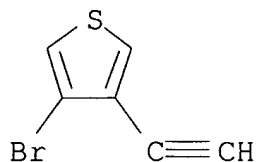
RN 225244-01-9 HCA

CN Thiophene, 3-bromo-4-ethynyl-, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 198491-48-4

CMF C6 H3 Br S



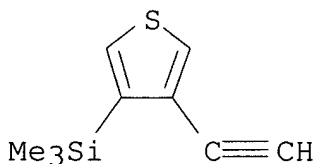
RN 225244-03-1 HCA

CN Silane, (4-ethynyl-3-thienyl)trimethyl-, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 176168-20-0

CMF C9 H12 S Si



IT **225244-01-9 225244-03-1**

(photocond. of substituted polyacetylene-based electrophotog. photoreceptors contg. under visible light exposure)

L37 ANSWER 9 OF 26 HCA COPYRIGHT 2005 ACS on STN

132:173261 Structure-Property Relationships for Photoconduction in Substituted Polyacetylenes. Tang, Ben Zhong; Chen, Hong Zheng; Xu, Rui Song; Lam, Jacky W. Y.; Cheuk, Kevin K. L.; Wong, Henry N. C.; Wang, Mang (Department of Chemistry and Center for Display Research, Hong Kong University of Science & Technology, Clear Water Bay Kowloon, Hong Kong). Chemistry of Materials, 12(1), 213-221 (English) 2000. CODEN: CMATEX. ISSN: 0897-4756. Publisher: American Chemical Society.

AB New photoconductive materials are explored from three groups of polyacetylenes: poly(phenylacetylenes) $-[HC:C(C_6H_5-p-R)]_n-$, poly(3-thienylacetylenes) $-[HC:C(3-C_4H_2S-\beta-R')]_n-$, and poly(1-alkynes) $-[HC:C[(CH_2)_mR'']]_n-$, where R = CH₃ (2), CO₂(CH₂)₆CO-Biph-OC₇H₁₅ (Biph = 4,4'-biphenyl; 3); R' = Si(CH₃)₃ (4), Br (5); and R'' = CO₂(CH₂)₆CO-Biph-OC₉H₁₉ (m = 2; 6), 9-carbazolyl (m = 3; 7) and OCO-Biph-OC₇H₁₅ (m = 9; 8).

Photoconduction in the polyacetylenes under illumination of visible light is investigated using photoinduced xerog. discharge technique. In the pure (undoped) state, all the polyacetylenes except 5 show higher photosensitivity than do poly(phenylacetylene) ($R = H$; 1), a well-studied photoconducting polyacetylene, and poly(9-vinylcarbazole), the best-known photoconducting vinyl polymer. Among the polyacetylenes, photoconduction performance of the polymers with electron-donating and/or hole-transporting moieties is superior to those with electron-accepting ones. The liq. cryst. polymer 6 exhibits very high photosensitivity, probably due to the formation of cryst. aggregates of its mesogenic pendants induced by the thermal treatment in the photoreceptor prepn. process. C60 acts as a photocond. enhancer when doped to amorphous 3, but functions as a crystallinity-breaking plasticizer when doped to liq. cryst. 6, leading to a large decrease in photocond. While 3 shows a low photosensitivity ($2.8 \times 10^{-3} \text{ lx}^{-1} \text{ s}^{-1}$) to a 573 nm light in the undoped state, doping with I2 and sensitization with Crystal violet (CV) dramatically increase its photosensitivity (up to $41.2 \times 10^{-3} \text{ lx}^{-1} \text{ s}^{-1}$). The CV-sensitized 4 exhibits high photocond. in the near-IR spectral region, which may find technol. applications in the digital photoimaging systems.

IT **225244-01-9 225244-03-1**

(photoconduction in electrophotog. photoreceptors of substituted polyacetylenes and doping/sensitizing- and morphol. effects on)

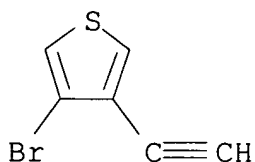
RN 225244-01-9 HCA

CN Thiophene, 3-bromo-4-ethynyl-, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 198491-48-4

CMF C6 H3 Br S



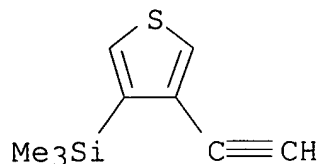
RN 225244-03-1 HCA

CN Silane, (4-ethynyl-3-thienyl)trimethyl-, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 176168-20-0

CMF C9 H12 S Si



IT **225244-01-9 225244-03-1**

(photoconduction in electrophotog. photoreceptors of substituted polyacetylenes and doping/sensitizing- and morphol. effects on)

L37 ANSWER 10 OF 26 HCA COPYRIGHT 2005 ACS on STN

132:166874 Photoconductivity of substituted polyacetylenes and their doped composites. Chen, H. Z.; Lam, J. W. Y.; Xu, R. S.; Wang, M.; Tang, B. Z. (Department of Polymer Science & Engineering, Zhejiang University, Hangzhou, 310027, Peop. Rep. China). Polymer Preprints (American Chemical Society, Division of Polymer Chemistry), 40(2), 651-652 (English) 1999. CODEN: ACPPAY. ISSN: 0032-3934. Publisher: American Chemical Society, Division of Polymer Chemistry.

AB The intrinsic photocond. and the doping effects of electron acceptor (C60 and I2) and electron donor (crystal violet) in substituted polyacetylenes are studied. All the polyacetylenes studied show photocond. 500-750 nm, and higher photosensitivity, except for one case. Pendent side chains play an important role in photocond. of substituted polyacetylenes, which is useful in the design and synthesis of substituted polyacetylenes with excellent photocond. There ate two effects of decline and enhancement of the photocond. in substituted polyacetylene upon C60 doping. The photocond. is improved regardless of whether the electron acceptor I2 or electron donor crystal violet is doped in polyacetylenes.

IT **225244-01-9 225244-03-1**

(Photocond. of substituted polyacetylenes and their doped composites)

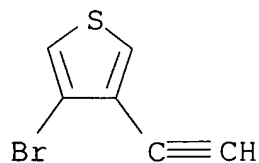
RN 225244-01-9 HCA

CN Thiophene, 3-bromo-4-ethynyl-, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 198491-48-4

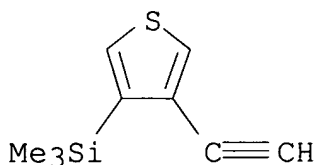
CMF C6 H3 Br S



RN 225244-03-1 HCA
 CN Silane, (4-ethynyl-3-thienyl)trimethyl-, homopolymer (9CI) (CA
 INDEX NAME)

CM 1

CRN 176168-20-0
 CMF C9 H12 S Si



IT **225244-01-9 225244-03-1**
 (Photocond. of substituted polyacetylenes and their doped
 composites)

L37 ANSWER 11 OF 26 HCA COPYRIGHT 2005 ACS on STN

131:45158 Thermal Behavior of Diynes with Formally Conjugated
 Heteroaromatic Sidegroups. Sarkar, Abhijit; Talwar, Satya S. (Dep.
 Chem., Indian Institute of Technology, Powai, Bombay, 400076,
 India). Bulletin of the Chemical Society of Japan, 72(4), 859-864
 (English) 1999. CODEN: BCSJA8. ISSN: 0009-2673. Publisher:
 Chemical Society of Japan.

AB Diynes with heteroarom. sidegroups directly linked to the acetylenic
 backbone were found to show liq. cryst. behavior upon heating.
 Thus, 1,4-di(2-thienyl)-1,3-butadiyne, 1,4-di(3-thienyl)-1,3-
 butadiyne, 1,4-di(3-benzo[b]thienyl)-1,3-butadiyne,
 1-(3-quinolyl)-4-(2-thienyl)-1,3-butadiyne, 1-(3-quinolyl)-4-(3-
 thienyl)-1,3-butadiyne, and 5-(2-thienyl)-2,4-pentadiyne-1-ol were
 investigated for their thermal behavior. These diynes also
 underwent polymn. in their liq. cryst. state, although the polymers
 so formed did not show liq. cryst. behavior. It was found that the
 S-atom of the heteroarom. moieties tends to play a role in making
 the diynes show liq. cryst. behavior. Differential scanning
 calorimetry, thermogravimetric anal. and hot stage microscopy were
 used to investigate the liq. cryst. nature of the diynes. All of
 them showed a nematic liq. cryst. phase upon annealing, whereas
 smectic phase was totally absent.

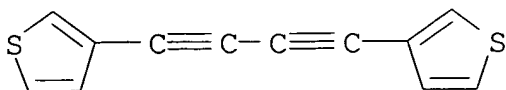
IT **135161-25-0P 227475-48-1P**
 (thermal behavior of diynes with formally conjugated heteroarom.
 sidegroups)

RN 135161-25-0 HCA
 CN Thiophene, 3,3'-(1,3-butadiyne-1,4-diyl)bis-, homopolymer (9CI) (CA
 INDEX NAME)

CM 1

CRN 81294-14-6

CMF C12 H6 S2



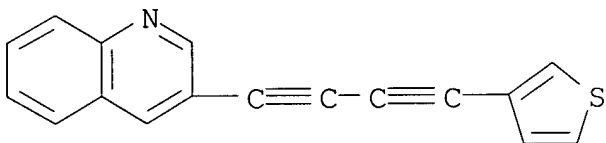
RN 227475-48-1 HCA

CN Quinoline, 3-[4-(3-thienyl)-1,3-butadiynyl]-, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 144091-95-2

CMF C17 H9 N S



IT **135161-25-0P 227475-48-1P**

(thermal behavior of diynes with formally conjugated heteroarom. sidegroups)

L37 ANSWER 12 OF 26 HCA COPYRIGHT 2005 ACS on STN

131:19393 Synthesis and optical properties of poly(thienylacetylenes). Tang, Ben-Zhong; Poon, Wan-Hong; Peng, Han; Nai-Ching Wong, Henry; Ye, Xin-Shan; Monde, Takashi (Department of Chemistry, Hong Kong University of Science and Technology, Hong Kong, Peop. Rep. China). Chinese Journal of Polymer Science, 17(1), 81-86 (English) 1999. CODEN: CJPSEG. ISSN: 0256-7679. Publisher: Springer-Verlag Singapore Pte. Ltd..

AB 3-Ethynyl-4-(trimethylsilyl)thiophene and 3-ethynyl-4-bromothiophene undergo selective polymn. through the acetylene group in the presence of MoCl5 and WCl6 - Ph3SiH catalysts to give sol., high-mol.-wt. poly(thienylacetylenes) (Mw up to 602,000) in high yields (up to 100%). The light transmission spectra of THF solns. of the polymers show a continuous red-shift with increasing concn. The photochromic effect shows a logarithmic dependence on concn., i.e., the optical transition of the polymers are predictable and tunable by simply changing the concn.

IT **225244-01-9P**, 3-Ethynyl-4-bromothiophene homopolymer
225244-03-1P, 3-Ethynyl-4-(trimethylsilyl)thiophene
 homopolymer
 (prepn. and concn. tunable optical transmission and chromism of
 poly(thienylacetylene) conjugated polymers)

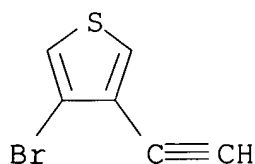
RN 225244-01-9 HCA

CN Thiophene, 3-bromo-4-ethynyl-, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 198491-48-4

CMF C6 H3 Br S



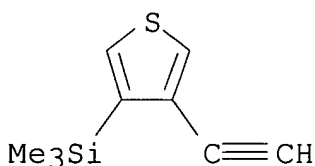
RN 225244-03-1 HCA

CN Silane, (4-ethynyl-3-thienyl)trimethyl-, homopolymer (9CI) (CA
 INDEX NAME)

CM 1

CRN 176168-20-0

CMF C9 H12 S Si



IT **225244-01-9P**, 3-Ethynyl-4-bromothiophene homopolymer
225244-03-1P, 3-Ethynyl-4-(trimethylsilyl)thiophene
 homopolymer

(prepn. and concn. tunable optical transmission and chromism of
 poly(thienylacetylene) conjugated polymers)

L37 ANSWER 13 OF 26 HCA COPYRIGHT 2005 ACS on STN

130:352670 Synthesis and characterization of poly(thienylacetylenes)
 with novel optical properties. Cha, John A.; Poon, Wan Hang; Peng,
 Han; Ye, Xie-Shan; Wong, Henry N. C.; Monde, Takashi; Tang, Ben
 Zhong (Department of Chemistry, Hong Kong University of Science and
 Technology, Hong Kong, Peop. Rep. China). Polymeric Materials

Science and Engineering, 80, 128-129 (English) 1999. CODEN: PMSEDG. ISSN: 0743-0515. Publisher: American Chemical Society.

AB Poly[3-(4-bromo)thienylacetylene] and poly[3-(4-trimethylsilyl)thienylacetylene] are prepd. from their resp. monomer in the presence of W- and Mo-triphenylsilane catalyst systems. The use of triphenylsilane co-catalyst effects selective polymn. of the acetylenic triple bond in the monomer while keeping the thiophene moiety intact as shown by IR and NMR characterization of the polymer products. Furthermore, the presence of triphenylsilane increases the polymer yield and decreases the polydispersity index. The optical transmission spectra of the polythienylacetylenes in THF display a characteristic shift towards longer wavelength with increasing polymer concn., with the cutoff wavelength empirically correlated to the polymer concn. This novel concentratochromic effect may be attributed to the interchain pi-pi interactions in the conjugated polymer backbones. Polythienylacetylenes with tunable optical properties may find applications as optical filters, switches, and limiters. Moreover, the concentratochromism may be used as a probe for measuring the extent of pi-pi interactions in conjugated polymer systems.

IT **225244-01-9P 225244-03-1P**

(synthesis and characterization of poly(thienylacetylenes) with novel optical properties)

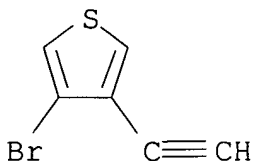
RN 225244-01-9 HCA

CN Thiophene, 3-bromo-4-ethynyl-, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 198491-48-4

CMF C6 H3 Br S



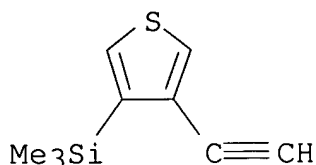
RN 225244-03-1 HCA

CN Silane, (4-ethynyl-3-thienyl)trimethyl-, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 176168-20-0

CMF C9 H12 S Si



IT **225244-01-9P 225244-03-1P**

(synthesis and characterization of poly(thienylacetylenes) with novel optical properties)

L37 ANSWER 14 OF 26 HCA COPYRIGHT 2005 ACS on STN

130:312179 Chemical and electrochemical polymerization of diacetylenes containing thienyl moiety as the side group. Sarkar, Abhijit; Talwar, Satya S.; Okada, Shuji; Nakanishi, Hachiro (Department Chemistry, Indian Institute Technology, Bombay, 400076, India). Polymer Bulletin (Berlin), 42(1), 69-76 (English) 1999. CODEN: POBUDR. ISSN: 0170-0839. Publisher: Springer-Verlag.

AB Two sym. diacetylene monomers contg. thienyl moiety as the side groups, namely 1,4-bis(2'-thienyl)butadiyne and 1,4-bis(3'-thienyl)butadiyne, are reported which were successfully polymd. electrochem. They were also polymd. chem. in soln. using Lewis acid as initiator. The resulting polymers were characterized by elemental anal., IR spectra, absorption spectra, and by solid-state NMR spectra. The polymers were found to have conjugated π -electron structure and both of them show high environmental stability. The properties of the polymers were compared with that of poly(3-methylthiophene) which is a conventional and much studied conjugated polymer. The elec. cond. of the polymers was also investigated.

IT **135161-25-0P**

(chem. and electrochem. polymn. of thienyl-contg. diacetylenes)

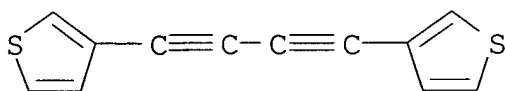
RN 135161-25-0 HCA

CN Thiophene, 3,3'-(1,3-butadiyne-1,4-diyl)bis-, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 81294-14-6

CMF C12 H6 S2



IT **135161-25-0P**

(chem. and electrochem. polymn. of thienyl-contg. diacetylenes)

L37 ANSWER 15 OF 26 HCA COPYRIGHT 2005 ACS on STN

129:28306 Synthesis of conjugated polymers by vapor deposition polymerization. Hsu, Chain-Shu; Lin, Ting-Li (Department of Applied Chemistry, National Chiao Tung University, Hsinchu, Taiwan). Materials Research Society Symposium Proceedings, 488(Electrical, Optical, and Magnetic Properties of Organic Solid-State Materials IV), 347-358 (English) 1998. CODEN: MRSPDH. ISSN: 0272-9172. Publisher: Materials Research Society.

AB The synthesis of poly(2,5-thienylene vinylene) and poly(4,7-thianaphthene) by vapor deposition polymn. is presented. 2,5-Di(bromomethyl)thiophene was subjected to vapor phase pyrolysis at 550 .degree.C to form a reactive intermediate. Upon condensation, the reactive intermediate polymd. spontaneously at a temp. higher than -25 .degree.C to produce poly(2,5-thienylene vinylene). The obtained poly(2,5-thienylene vinylene)s were fractionated into THF sol. and insol. fractions. The no. av. mol. wts. of the THF sol. fractions range from 1500 to 4000 as detd. by GPC measurements. The obtained polymer shows no glass transition and m.p. on the DSC scans. Doping of a poly(2,5-thienylene vinylene) film with I2 vapor led to a cond. of 1×10^{-4} S cm⁻¹. In the second part of this study, 2,3-diethynylthiophene was subjected to vapor phase pyrolysis at 300 .degree.C to yield a reactive intermediate, 4,7-dehydrothianaphthene. Upon condensation, the obtained 4,7-dehydrothianaphthenene was polymd. spontaneously at a temp. higher than -25 .degree.C to produce poly(4,7-thianaphthene). The obtained poly(4,7-thianaphthene) was insol. in common lab. solvents and shows also no m.p. and glass transition on the DSC scans.

IT 208053-53-6P

(poly(4,7-thianaphthene); synthesis and characterization of poly(2,5-thienylene vinylene) and poly(4,7-thianaphthene) by vapor deposition polymn.)

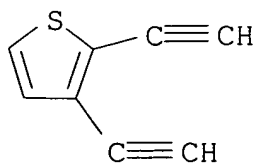
RN 208053-53-6 HCA

CN Thiophene, 2,3-diethynyl-, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 153143-04-5

CMF C8 H4 S



IT 208053-53-6P

(poly(4,7-thianaphthene); synthesis and characterization of poly(2,5-thienylene vinylene) and poly(4,7-thianaphthene) by vapor deposition polymn.)

L37 ANSWER 16 OF 26 HCA COPYRIGHT 2005 ACS on STN

127:359196 Synthesis of polyphenylene derivatives by thermolysis of enediynes and dialkynylaromatic monomers. John, Jens A.; Tour, James M. (Dep. Chem. Biochem., Univ. South Carolina, Columbia, SC, 29208, USA). Tetrahedron, 53(45), 15515-15534 (English) 1997. CODEN: TETRAB. ISSN: 0040-4020. Publisher: Elsevier.

AB Substituted enediynes and dialkynyl aroms. were prepd. using Pd- or Pd/Cu-catalyzed cross coupling procedures, to obtain monomers that were subjected to thermal polymn. to afford the corresponding poly(p-phenylene)s, poly(1,4-naphthalene)s, poly(benzo[c]thiophene)s, and poly(dibenzothiophene)s. The scope of the polymn. process is illustrated based upon substituent patterns and cyclization. moieties. The superb thermal resiliency of the polyphenylenes and Polythiophenylenes obtained was demonstrated using thermogravimetric anal. The polymer structure was generally confirmed using IR data correlations to small mols. that resembled the polymer repeating unit structure. Radical trapping of dimeric intermediates, that were analyzed by GC/MS, further substantiated the proposed mechanistic route. The step-growth polymn. as monitored by GC/MS, further substantiated the proposed mechanistic route. The step-growth polymn. pattern was detd. by monitoring the degree of monomer consumption vs. the polymer mol. wt. The method is particularly well-suited for polymn. since it requires no exogenous chem. catalysts or reagents for the process, and it is a non-condensation process wherein no volatile byproducts are formed in the polymn. reaction, which makes it amenable to polymer film-forming vapor deposition processes, for, e.g., fabrication of semiconductor devices.

IT 198693-72-0P, 3-(2'-Phenylethynyl)-4-ethynylthiophene homopolymer

(prepn. and high-temp. stability of polyphenylenes and polybenzothiophenes by thermolysis of enediynes and dialkynyl arom. monomers)

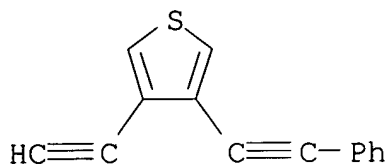
RN 198693-72-0 HCA

CN Thiophene, 3-ethynyl-4-(phenylethynyl)-, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 198693-59-3

CMF C14 H8 S



IT **198693-72-0P**, 3-(2'-Phenylethynyl)-4-ethynylthiophene homopolymer
(prepn. and high-temp. stability of polyphenylenes and polybenzothiophenes by thermolysis of enediynes and dialkynyl arom. monomers)

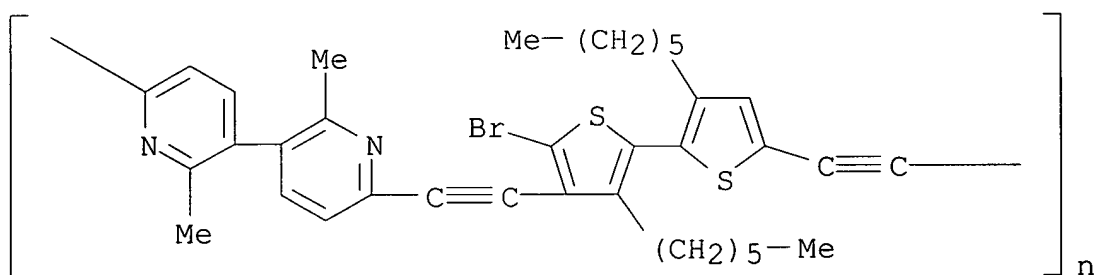
L37 ANSWER 17 OF 26 HCA COPYRIGHT 2005 ACS on STN
125:342351 Nonlinear optical materials and apparatus. Ooba, Naoki; Kaino, Toshikuni; Tomaru, Akira (Nippon Telegraph & Telephone, Japan). Jpn. Kokai Tokkyo Koho JP 08220574 A2 19960830 Heisei, 12 pp. (Japanese). CODEN: JKXXAF. APPLICATION: JP 1995-50307 19950216.

AB A fast broadband nonlinear material comprises a polyarylene ethynylene (Ar)_nC.tplbond.C(Ar')_mC.tplbond.C, where Ar, Ar' = (un)substituted arom. donor and acceptor ring with respect to conjugate system, resp.; n, m = 1-6; and n and/or m .gtoreq.2.

IT **183596-80-7**
(third-order nonlinear optical materials and app.)

RN 183596-80-7 HCA

CN Poly[(2,2'-dimethyl[3,3'-bipyridine]-6,6'-diyl)-1,2-ethynediyl(5-bromo-3,3'-dihexyl[2,2'-bithiophene]-4,5'-diyl)-1,2-ethynediyl]
(9CI) (CA INDEX NAME)



IT **183596-80-7**
(third-order nonlinear optical materials and app.)

L37 ANSWER 18 OF 26 HCA COPYRIGHT 2005 ACS on STN
124:203332 Preparation of electrically conducting polyenes by polymerization of ethynylthiophenes and optionally comonomers. Naarmann, Herbert (BASF A.-G., Germany). Ger. Offen. DE 4424711 A1 19960118, 6 pp. (German). CODEN: GWXXBX. APPLICATION: DE

1994-4424711 19940713.

AB The title polymers are prepd. in the form of porous films, fibers, etc. Polymn. of 2-ethynylthiophene in propylene carbonate contg. Bu₄NPF₆ by anodic oxidn. in an electrochem. cell gave a porous polymer film showing elec. cond. 50 S/cm².

IT **97418-70-7P**, Poly(3-ethynylthiophene) **174672-62-9P**
, Poly(3,4-diethynylthiophene)
(electrochem. polymn. for prepn. of porous elec. conductors)

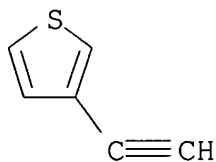
RN 97418-70-7 HCA

CN Thiophene, 3-ethynyl-, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 67237-53-0

CMF C6 H4 S



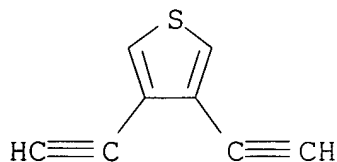
RN 174672-62-9 HCA

CN Thiophene, 3,4-diethynyl-, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 138354-60-6

CMF C8 H4 S



IT **97418-70-7P**, Poly(3-ethynylthiophene) **174672-62-9P**
, Poly(3,4-diethynylthiophene)
(electrochem. polymn. for prepn. of porous elec. conductors)

L37 ANSWER 19 OF 26 HCA COPYRIGHT 2005 ACS on STN

122:10872 Polymerization of 1,4-bis(2-thienyl)-1,3-butadiyne and 1,4-bis(3-thienyl)-1,3-butadiyne. Sarkar, Abhijit; Sachdeva, Rakesh; Talwar, Satya S. (Dep. Chem., Indian Inst. Technol., Bombay, 400 076, India). Polym. Sci., Volume 1, 278-83. Editor(s): Bhardwaj, I. S. Allied Publ.: New Delhi, India. (English) 1994.

CODEN: 60AIAY.

AB Thiophene derivs. contg. diacetylenic units, i.e., 1,4-bis(2-thienyl)-1,3-butadiyne and 1,4-bis(3-thienyl)-1,3-butadiyne, were electrochem. and chem. polymd. The resulting polymers were characterized by elemental anal., IR spectra and absorption spectra. The polymers showed high environmental stability and, although they did not show any significant elec. cond., the UV-visible spectra and doping expts. indicated that modification towards getting a low band gap semiconductor is a possibility for this category of polymers.

IT **135161-25-0P**, 1,4-Bis(3-thienyl)-1,3-butadiyne homopolymer (prepn. and characterization of)

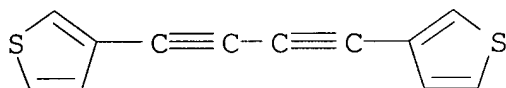
RN 135161-25-0 HCA

CN Thiophene, 3,3'-(1,3-butadiyne-1,4-diyl)bis-, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 81294-14-6

CMF C12 H6 S2



IT **135161-25-0P**, 1,4-Bis(3-thienyl)-1,3-butadiyne homopolymer (prepn. and characterization of)

L37 ANSWER 20 OF 26 HCA COPYRIGHT 2005 ACS on STN

121:10145 Polyheterocycles containing alkene spacer linkages. Part I. Synthesis and electropolymerization of 3-styrylthiophenes. Smith, J. R.; Campbell, S. A.; Ratcliffe, N. M.; Dunleavy, M. (Applied Electrochemistry Group, Department of Chemistry, University of Portsmouth, White Swan Road, Portsmouth, PO1 2DT, UK). Synthetic Metals, 63(3), 233-43 (English) 1994. CODEN: SYMEDZ. ISSN: 0379-6779.

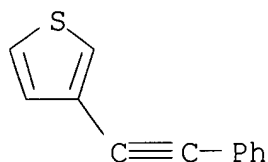
AB The synthesis and electrochem. behavior of novel thiophene compds. contg. a substituted Ph group sepd. by an alkene spacer are described. In such systems, it was proposed that the mol. geometry should allow the .pi.-electron d. of the Ph group to be delocalized with that of the thiophene ring by means of the alkene spacer. The presence of this unsatd. linkage should also minimize steric hindrance between the two rings. A no. of such monomers exhibiting a range of electronic effects were prepd. and their electrochem. behavior investigated. Although films were deposited on the anode surface by electropolymn., the conductivities were of the order of 10⁻⁶ S cm⁻¹. The nature of the films was investigated by

electrochem. and microscopic techniques. Potentiodynamic studies indicated that the alkene spacer linkage may be subject to irreversible electrooxidn. Polymer redox peaks, characteristic of anion mobility within conductive polymers, were absent from the cyclic voltammograms. SEM observations showed that the films were exceptionally smooth and homogeneous.

IT **155827-44-4P**, 3-(Phenylethynyl)thiophene homopolymer
(films, electrochem. prepn. and properties of)
RN 155827-44-4 HCA
CN Thiophene, 3-(phenylethynyl)-, homopolymer (9CI) (CA INDEX NAME)

CM 1

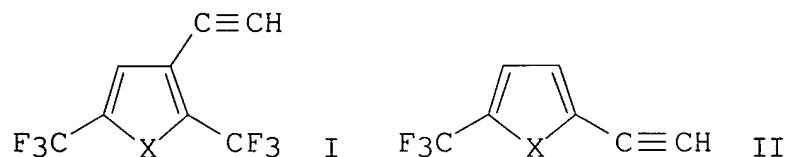
CRN 131423-29-5
CMF C12 H8 S



IT **155827-44-4P**, 3-(Phenylethynyl)thiophene homopolymer
(films, electrochem. prepn. and properties of)

L37 ANSWER 21 OF 26 HCA COPYRIGHT 2005 ACS on STN
119:160851 Syntheses of acetylenes containing trifluoromethyl substituted heterocyclic ring. Muramatsu, Hiroshige; Shibata, Katsuyoshi; Matsui, Masaki (Fac. Eng., Gifu Univ., Gifu, 501-11, Japan). Kenkyu Hokoku - Asahi Garasu Zaidan, 60, 167-74 (Japanese) 1992. CODEN: KHAZE2. ISSN: 0916-7064.

GI



AB Trifluoromethylated heterocyclics I (X = O, S) and II (X = O, S) were prepd. Fluorination of the 2,5-dicarboxylic acid of furan and thiophene with SF₄HF afforded 2,5-bis(trifluoromethyl) derivs., together with 5-(trifluoromethyl)-2-carboxylic acids, which were decarboxylated by heating with Cu. Treating the mono and

bis(trifluoromethyl) derivs. with BuLi and CF₂:CCl₂ gave dichlorofluorvinyl derivs. which with EtLi in quinoline gave II and I, resp. Polymn. of I using WCl₆-Ph₄Sn as catalyst gave high-mol.-wt. polyacetylenes, whereas II did not polymerize. Thermal decompn. and gas permeability (O, N, CO, CH₄, and CO₂) of the polymers were measured. Absorption spectra were presented.

IT **127798-28-1P**

(prepn. and thermal properties and permeability of)

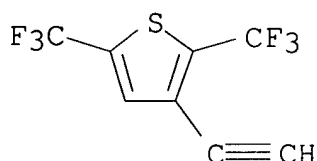
RN 127798-28-1 HCA

CN Thiophene, 3-ethynyl-2,5-bis(trifluoromethyl)-, homopolymer (9CI)
(CA INDEX NAME)

CM 1

CRN 127798-27-0

CMF C8 H2 F6 S



IT **127798-28-1P**

(prepn. and thermal properties and permeability of)

L37 ANSWER 22 OF 26 HCA COPYRIGHT 2005 ACS on STN

117:71160 Preparation and properties of polyacetylene membranes substituted with trifluoromethylated heterocyclic groups. Hayakawa, Yoshio; Nishida, Masakazu; Okumura, Akinori; Matsui, Masaki; Muramatsu, Hiroshige (Gov. Ind. Res. Inst. Nagoya, Nagoya, 462, Japan). Polymer Bulletin (Berlin, Germany), 28(3), 293-9 (English) 1992. CODEN: POBUDR. ISSN: 0170-0839.

AB Membranes of poly[2,5-bis(trifluoromethyl)-3-ethynylthiophene] and poly[2,5-bis(trifluoromethyl)-3-ethynylfuran] were prepd. and their properties were evaluated. They were highly gas permeable, and showed somewhat low liq. permeability and preferential permeation of H₂O in a pervaporation of aq. alc.

IT **127798-28-1**

(membranes, surface tension and permeation of)

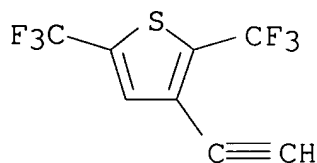
RN 127798-28-1 HCA

CN Thiophene, 3-ethynyl-2,5-bis(trifluoromethyl)-, homopolymer (9CI)
(CA INDEX NAME)

CM 1

CRN 127798-27-0

CMF C8 H2 F6 S



IT **127798-28-1**

(membranes, surface tension and permeation of)

L37 ANSWER 23 OF 26 HCA COPYRIGHT 2005 ACS on STN

115:93047 Solid-state and electrochemical polymerization of novel diacetylene monomers. Sarkar, Abhijit; Kulkarni, Anuradha; Contractor, A. Q.; Talwar, S. S. (Dep. Chem., Indian Inst. Technol., Bombay, 400 076, India). Polym. Sci., [Symp. Proc. Polym. '91], Volume 1, 267-72. Editor(s): Sivaram, S. Tata McGraw-Hill: New Delhi, India. (English) 1991. CODEN: 57CFA3.

AB Solid-state polymn. of 2 sym. disubstituted diacetylenes, 1,4-bis(2-thienyl)-1,3-butadiyne and 1,4-bis(3-thienyl)-1,3-butadiyne (I) is reported. Both the monomers are moderately reactive towards solid-state polymn. Preliminary single-crystal x-ray data justify their low reactivity. DSC spectra of both the monomers show liq.-cryst. phases. Electrochem. polymn. of I resulted in a polymer which had a golden metallic luster.

IT **135161-25-0P**

(prepn. and characterization of)

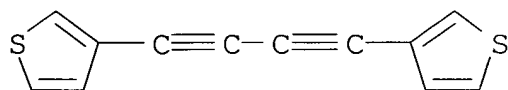
RN 135161-25-0 HCA

CN Thiophene, 3,3'-(1,3-butadiyne-1,4-diyl)bis-, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 81294-14-6

CMF C12 H6 S2



IT **135161-25-0P**

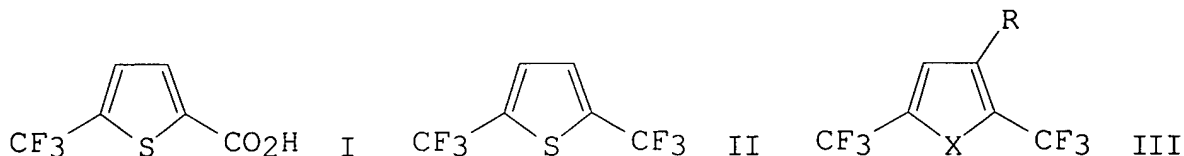
(prepn. and characterization of)

L37 ANSWER 24 OF 26 HCA COPYRIGHT 2005 ACS on STN

113:40370 Synthesis and polymerization of ethynylthiophenes and ethynylfurans containing trifluoromethyl groups. Nishida, Masakazu;

Fujii, Shozo; Aoki, Toshiki; Hayakawa, Yoshio; Muramatsu, Hiroshige; Morita, Tomohiko (Gov. Ind. Res. Inst., Nagoya, 462, Japan). Journal of Fluorine Chemistry, 46(3), 445-59 (English) 1990. CODEN: JFLCAR. ISSN: 0022-1139. OTHER SOURCES: CASREACT 113:40370.

GI



AB Fluorination of 2,5-thiophenedicarboxylic acid with SF₄ in the presence of anhyd. HF provided mono- and bis(trifluoromethyl)thiophenes I and II in moderate yields. Ethynylthiophenes and ethynylfurans, e.g., III (X = S, O; R = C.tplbond.CH) contg. CF₃ groups were prepd. via 2,2-dichloro-1-fluorovinyl compds., e.g., III (R = CF:CCl₂). In transition metal-catalyzed polymns., 3-ethynylthiophenes gave polymers in high yields, which were sol. in THF and/or fluorocarbons, while 2-ethynylthiophenes gave low yields of polymer. In .gamma.-ray induced polymn., only 2,5-bis(trifluoromethyl)-3-ethynylthiophene afforded the corresponding polymer. The presence of CF₃ as well as Me groups increased the thermal decompn. temps. of the polymers obtained.

IT **97418-70-7P 127798-28-1P 127798-30-5P**
(prepn. of)

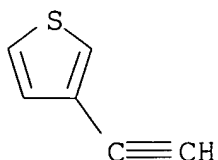
RN 97418-70-7 HCA

CN Thiophene, 3-ethynyl-, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 67237-53-0

CMF C6 H4 S



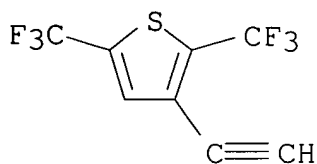
RN 127798-28-1 HCA

CN Thiophene, 3-ethynyl-2,5-bis(trifluoromethyl)-, homopolymer (9CI)
(CA INDEX NAME)

CM 1

CRN 127798-27-0

CMF C8 H2 F6 S



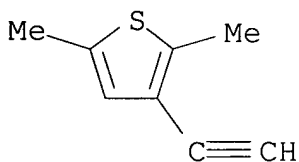
RN 127798-30-5 HCA

CN Thiophene, 3-ethynyl-2,5-dimethyl-, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 127798-29-2

CMF C8 H8 S



IT **97418-70-7P 127798-28-1P 127798-30-5P**
(prepn. of)

L37 ANSWER 25 OF 26 HCA COPYRIGHT 2005 ACS on STN
106:33532 Preparation and electrical properties of poly(3-thienylacetylene). Tanaka, Susumu; Okuhara, Kunio; Kaeriyama, Kyoji (Res. Inst. Polym. Text., Tsukuba, 305, Japan). Makromolekulare Chemie, 187(12), 2793-800 (English) 1986. CODEN: MACEAK. ISSN: 0025-116X.

AB 3-Thienylacetylene (I) [67237-53-0] was prepd. by reaction of 3-(2,2-dichloro-1-fluorovinyl)thiophene [106110-86-5] with BuLi in a 1:2 mol ratio, and subsequent hydrolysis. Polymn. of I with WCl6 and Ph4Sn [595-90-4] gave poly(3-thienylacetylene) (II) [**97418-70-7**], which contained a small amt. of benzene-insol. product. On heating II no wt. loss was obsd. up to 240.degree.. At 500.degree. the wt. loss was 18%. In differential scanning calorimetry, an exothermic peak appeared at 245.degree.. A pressed pellet, doped with iodine, exhibited cond. of .apprx.10⁻³ S/cm. The absorption spectrum of II showed a shoulder at 225 nm, a max.

absorption at 360 nm, and tailing up to .apprx.660 nm. In a soln. of II and iodine, a new absorption appeared in the near-IR region, but failed to develop enough to suggest high cond. of II doped with iodine. The electrochem. doping of II and electrochem. polymn. of I gave no conducting products.

IT **97418-70-7P**

(prepn. and elec. cond. of iodine-doped)

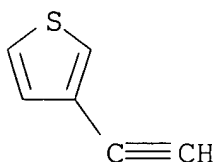
RN 97418-70-7 HCA

CN Thiophene, 3-ethynyl-, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 67237-53-0

CMF C6 H4 S



IT **97418-70-7P**

(prepn. and elec. cond. of iodine-doped)

L37 ANSWER 26 OF 26 HCA COPYRIGHT 2005 ACS on STN

103:54875 Acetylene polymers. (Mitsubishi Chemical Industries Co., Ltd., Japan). Jpn. Kokai Tokkyo Koho JP 60063212 A2 19850411 Showa, 5 pp. (Japanese). CODEN: JKXXAF. APPLICATION: JP 1983-172393 19830919.

AB Acetylene polymers with good oxidn. stability and heat resistance consist of structural repeating units CH:CR [R = 4-(PhS)C₆H₄, 4-(PhSO₂)C₆H₄, 2-thienyl, 3-thienyl, 4-(Ph₂NN:CH)C₆H₄]. Thus, a catalyst slurry contg. WCl₆ and Ph₄Sn was added to a soln. of 4-(PhSC₆H₄C.tplbond.CH in PhMe and stirred 24 h at room temp. to give an acetylene polymer [97418-75-2] which when doped with NOSbF₆ showed good elec. cond. for 3 mo. at atm. pressure in a desiccator.

IT **97418-70-7P**

(prepn. of, heat- and oxidn.-resistant)

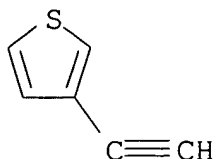
RN 97418-70-7 HCA

CN Thiophene, 3-ethynyl-, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 67237-53-0

CMF C6 H4 S

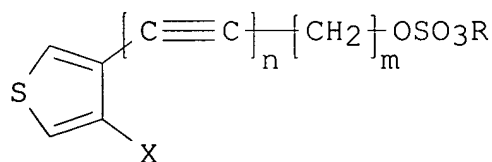


IT **97418-70-7P**
(prepn. of, heat- and oxidn.-resistant)

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L40 ANSWER 1 OF 18 HCA COPYRIGHT 2005 ACS on STN
142:198490 Oxidatively polymerizable sulfoxyalkynylthiophenes for
.pi.-conjugated electrically conducting polymers for electron-beam
lithography, and their manufacture. Suzuki, Hideo (Nissan Chemical
Industries, Ltd., Japan). Jpn. Kokai Tokkyo Koho JP 2005035955 A2
20050210, 12 pp. (Japanese). CODEN: JKXXAF. APPLICATION: JP
2003-276409 20030718.

GI



I

AB The sulfoxyalkynylthiophenes are I [X = halo,
(C.tplbond.C)n(CH2)mOSO3R; R = H, alkali metal, alk. earth metal; m,
n = 1-3]. Thus, 3,4-dibromothiophene was treated with
CH.tplbond.CCH2OH to give 3-(4-bromo-thiophen-3-yl)-prop-2-yn-1-ol
(II) and 3-[4-(3-hydroxy-propyn-1-yl)-thiophen-3-yl]-prop-2-yn-1-ol.
Then, II was sulfonated with SO3-DMF complex and treated with NaHCO3
to give I (X = Br, R = Na, m = n = 1).

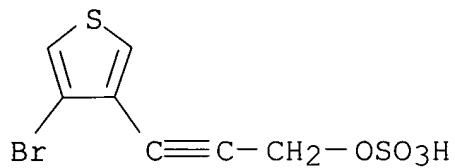
IT **835886-97-0P 835886-99-2P 835887-01-9P**
(manuf. of oxidatively polymerizable sulfoxyalkynylthiophenes for
conjugated elec. conducting polymers for electron-beam lithog.)

RN 835886-97-0 HCA

CN 2-Propyn-1-ol, 3-(4-bromo-3-thienyl)-, hydrogen sulfate, compd. with
pyridine (1:1) (9CI) (CA INDEX NAME)

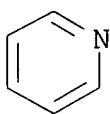
CM 1

CRN 835886-96-9
CMF C7 H5 Br O4 S2

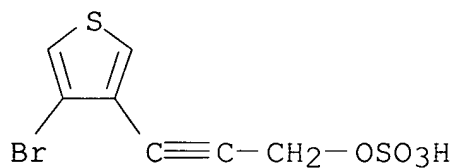


CM 2

CRN 110-86-1
CMF C5 H5 N

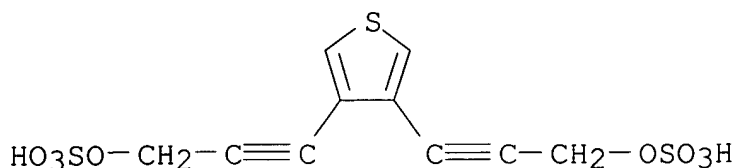


RN 835886-99-2 HCA
CN 2-Propyn-1-ol, 3-(4-bromo-3-thienyl)-, hydrogen sulfate, sodium salt
(9CI) (CA INDEX NAME)



● Na

RN 835887-01-9 HCA
CN 2-Propyn-1-ol, 3,3'-(3,4-thiophenediyl)bis-, bis(hydrogen sulfate),
disodium salt (9CI) (CA INDEX NAME)



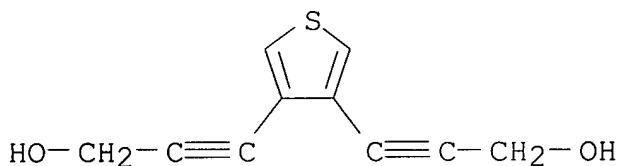
●2 Na

IT **330595-69-2P 835886-93-6P**

(manuf. of oxidatively polymerizable sulfoxyalkynylthiophenes for conjugated elec. conducting polymers for electron-beam lithog.)

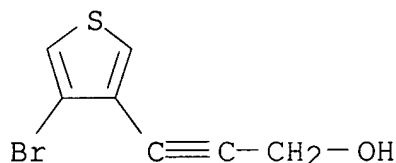
RN 330595-69-2 HCA

CN 2-Propyn-1-ol, 3,3'-(3,4-thiophenediyl)bis- (9CI) (CA INDEX NAME)



RN 835886-93-6 HCA

CN 2-Propyn-1-ol, 3-(4-bromo-3-thienyl)- (9CI) (CA INDEX NAME)



IC ICM C07D333-02

ICS C08F038-00; H01L021-027

CC 35-2 (Chemistry of Synthetic High Polymers)

Section cross-reference(s): 27, 74

IT **Conducting polymers**

(polythiophenes; manuf. of oxidatively polymerizable sulfoxyalkynylthiophenes for conjugated elec. conducting polymers for electron-beam lithog.)

IT **835886-97-0P 835886-99-2P 835887-01-9P**

(manuf. of oxidatively polymerizable sulfoxyalkynylthiophenes for conjugated elec. conducting polymers for electron-beam lithog.)

IT **330595-69-2P 835886-93-6P**

(manuf. of oxidatively polymerizable sulfoxyalkynylthiophenes for

conjugated elec. conducting polymers for electron-beam lithog.)

L40 ANSWER 2 OF 18 HCA COPYRIGHT 2005 ACS on STN

142:114604 Synthesis and Electrolytic Polymerization of the Ethylenedioxy-Substituted Terthiophene-Fullerene Dyad. Yamazaki, Tetsuya; Murata, Yasujiro; Komatsu, Koichi; Furukawa, Kazuaki; Morita, Masao; Maruyama, Norihiko; Yamao, Takeshi; Fujita, Shizuo (Institute for Chemical Research, Kyoto University, Uji, Kyoto, 611-0011, Japan). Organic Letters, 6(26), 4865-4868 (English) 2004. CODEN: ORLEF7. ISSN: 1523-7060. OTHER SOURCES: CASREACT 142:114604. Publisher: American Chemical Society.

GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Two derivs. of ethylenedioxy-substituted terthiophene-fullerene dyads were newly synthesized as the precursors for polythiophene having fullerene side chains. By electrolytic oxidn. of dyad I, the charm-bracelet type polythiophene, poly-(I), was obtained as a purple film, which showed electrochem. activity, electrochromism, and photoelectronic response.

IT **665003-42-9P**

(monomer; synthesis and electrolytic polymn. of ethylenedioxy-substituted terthiophene-fullerene dyad)

RN 665003-42-9 HCA

CN Thieno[3,4-b]-1,4-dioxin, 5,5'-[3-[(9-methyl[5,6]fulleren-C60-Ih-1(9H)-yl)ethynyl]-2,5-thiophenediyl]bis[2,3-dihydro- (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

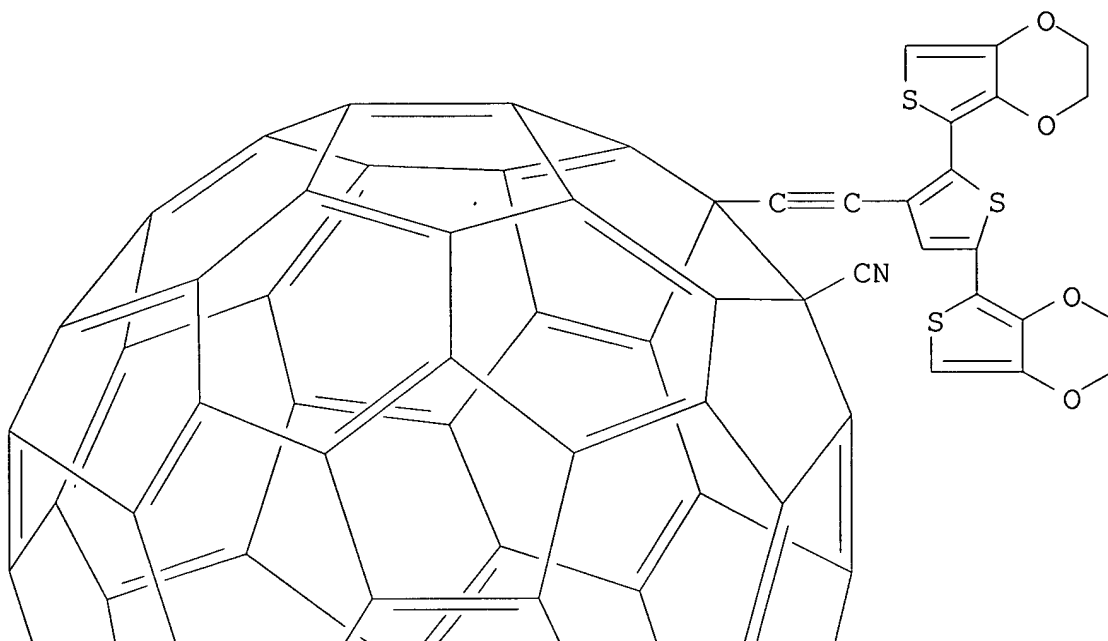
IT **765900-24-1P**

(synthesis and electrolytic polymn. of ethylenedioxy-substituted terthiophene-fullerene dyad)

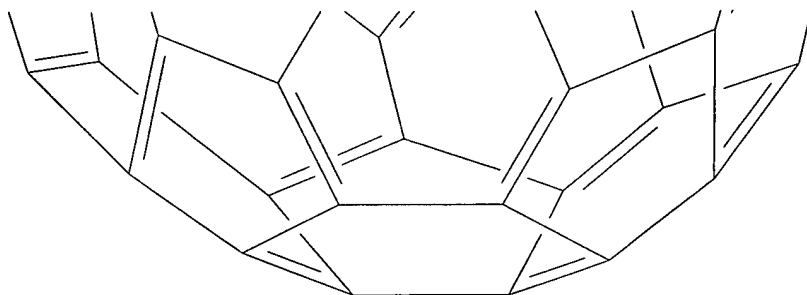
RN 765900-24-1 HCA

CN [5,6]Fullerene-C60-Ih-1(9H)-carbonitrile, 9-[[2,5-bis(2,3-dihydrothieno[3,4-b]-1,4-dioxin-5-yl)-3-thienyl]ethynyl]- (9CI) (CA INDEX NAME)

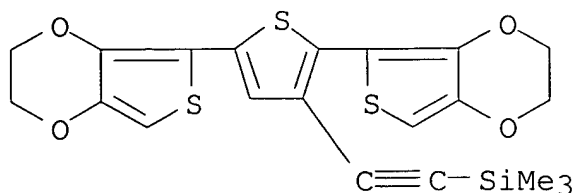
PAGE 1-A



PAGE 2-A

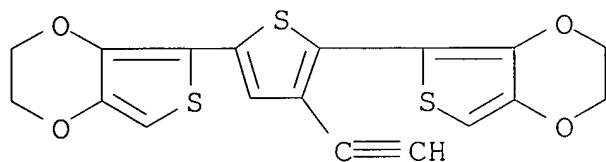


IT **765900-18-3P 765900-19-4P**
 (synthesis and electrolytic polymn. of ethylenedioxy-substituted
 terthiophene-fullerene dyad)
 RN 765900-18-3 HCA
 CN Silane, [[2,5-bis(2,3-dihydrothieno[3,4-b]-1,4-dioxin-5-yl)-3-
 thienyl]ethynyl]trimethyl- (9CI) (CA INDEX NAME)



RN 765900-19-4 HCA

CN Thieno[3,4-b]-1,4-dioxin, 5,5'-(3-ethynyl-2,5-thiophenediyl)bis[2,3-dihydro- (9CI) (CA INDEX NAME)



CC 35-7 (Chemistry of Synthetic High Polymers)
Section cross-reference(s): 72, 76

IT **Conducting polymers**

(polythiophenes; synthesis and electrolytic polymn. of ethylenedioxy-substituted terthiophene-fullerene dyad)

IT **665003-42-9P**

(monomer; synthesis and electrolytic polymn. of ethylenedioxy-substituted terthiophene-fullerene dyad)

IT **765900-24-1P**

(synthesis and electrolytic polymn. of ethylenedioxy-substituted terthiophene-fullerene dyad)

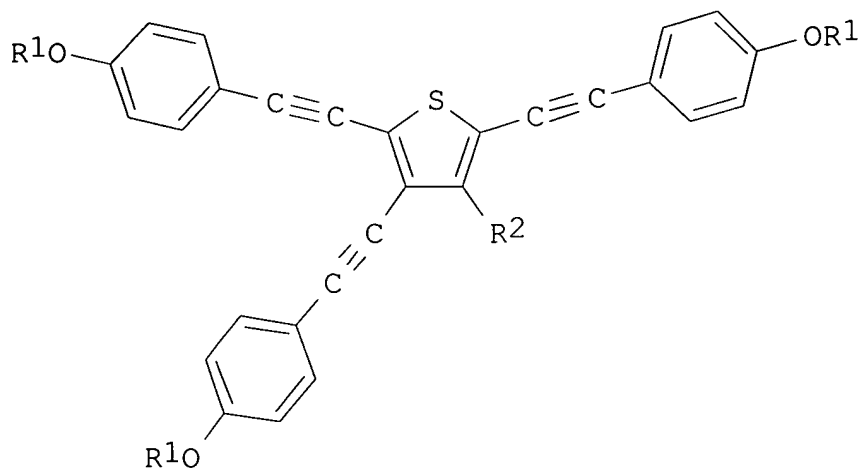
IT 765900-17-2P **765900-18-3P** **765900-19-4P**

(synthesis and electrolytic polymn. of ethylenedioxy-substituted terthiophene-fullerene dyad)

L40 ANSWER 3 OF 18 HCA COPYRIGHT 2005 ACS on STN

141:140264 Synthesis and Mesomorphic Properties of Multiynylthiophenes: 2,3,4,5-Tetrakis(4-alkoxyphenylethynyl)thiophenes and 2,3,5-Tris(4-alkoxyphenylethynyl)thiophenes. Hsu, Hsiu-Fu; Kuo, Chung-Hao; Chen, Chien-Fon; Lin, Yi-Hui; Huang, Li-Ya; Chen, Chien-Hsing; Cheng, Ko-Ching; Chen, Hsiu-Hui (Department of Chemistry, Tamkang University, Tamsui, 25137, Taiwan). Chemistry of Materials, 16(12), 2379-2385 (English) 2004. CODEN: CMATEX. ISSN: 0897-4756. OTHER SOURCES: CASREACT 141:140264. Publisher: American Chemical Society.

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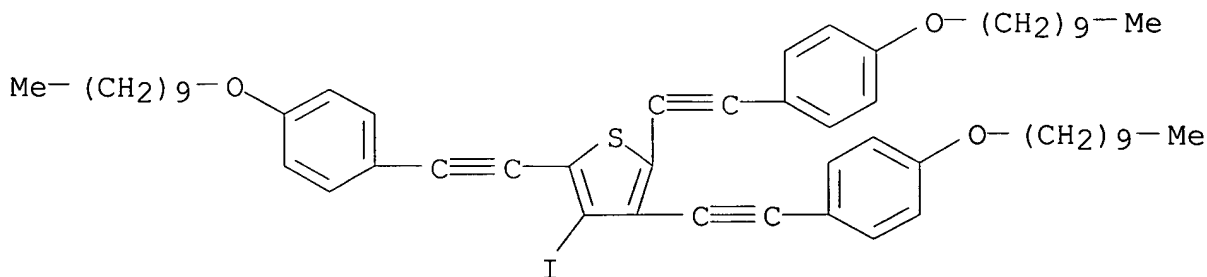
AB The synthesis and characterization of multiynylthiophenes, tetrakis(4-alkoxyphenylethynyl)thiophenes I [R1 = Bu, n-hexyl, n-octyl, n-decyl, n-dodecyl; R2 = 4-(R1O)C6H4C.tplbond.C] and tris(4-alkoxyphenylethynyl)thiophenes I (R2 = iodo), are reported, and their structure-mesomorphism relationship is discussed. The tetraynyl series I [R2 = 4-(R1O)C6H4C.tplbond.C] with a trapezoid core do not show any liq.-cryst. properties. With one less peripheral arm, series I (R2 = iodo) compds. are of the Y-shape geometry with rigid linear spacers, and nematic phases are obsd. for the octyloxy, decyloxy, and dodecyloxy derivs. Although the dipole-dipole interactions, desymmetrization, and disparity of the mesogenic cores can be accountable for their corresponding mesomorphic behaviors, the formation of the nematic phases of I (R2 = iodo) may be most likely attributed to the shape disparity of these two series of compds.

IT **727705-59-1P**

(prepn., mol. geometry and thermal and mesomorphic properties of poly(alkoxyphenylethynyl)thiophenes)

RN 727705-59-1 HCA

CN Thiophene, 2,3,5-tris[[4-(decyloxy)phenyl]ethynyl]-4-iodo- (9CI)
(CA INDEX NAME)

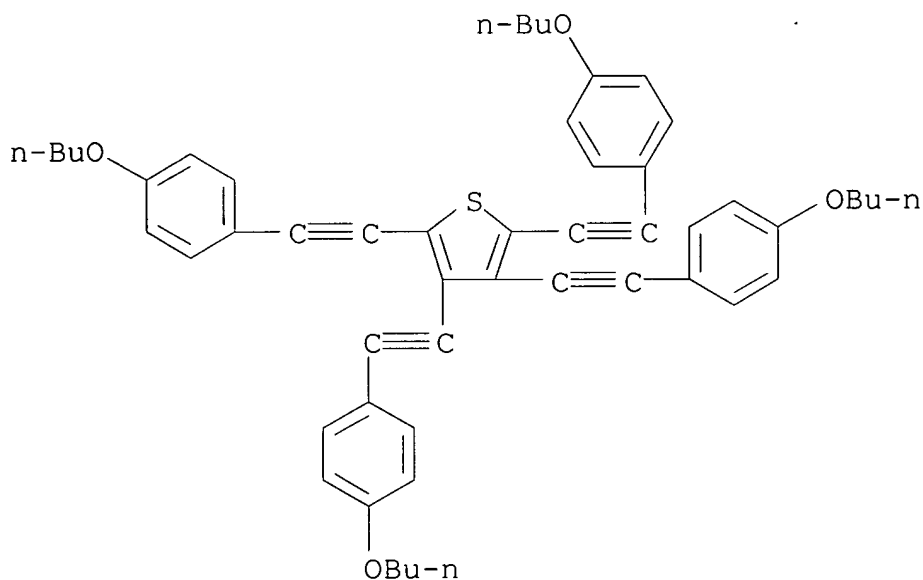


IT 727705-51-3P 727705-52-4P 727705-53-5P
 727705-54-6P 727705-55-7P 727705-56-8P
 727705-57-9P 727705-58-0P 727705-60-4P
 727705-61-5P 727705-62-6P

(prepn., mol. geometry and thermal and mesomorphic properties of
 poly(alkoxyphenylethynyl)thiophenes)

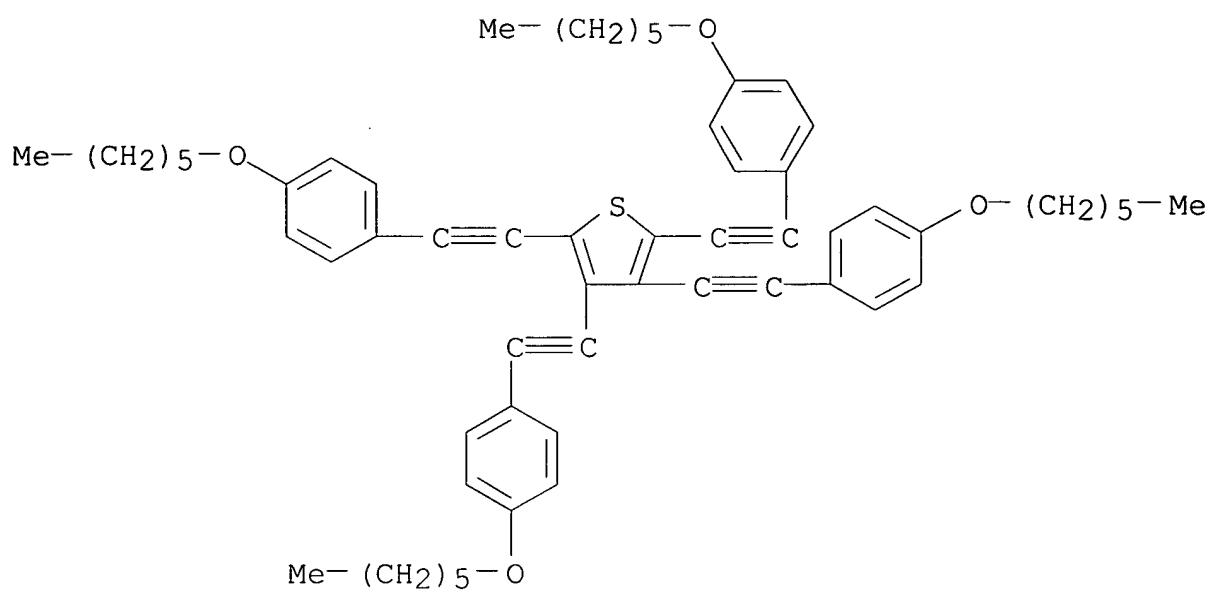
RN 727705-51-3 HCA

CN Thiophene, tetrakis[(4-butoxyphenyl)ethynyl]- (9CI) (CA INDEX NAME)



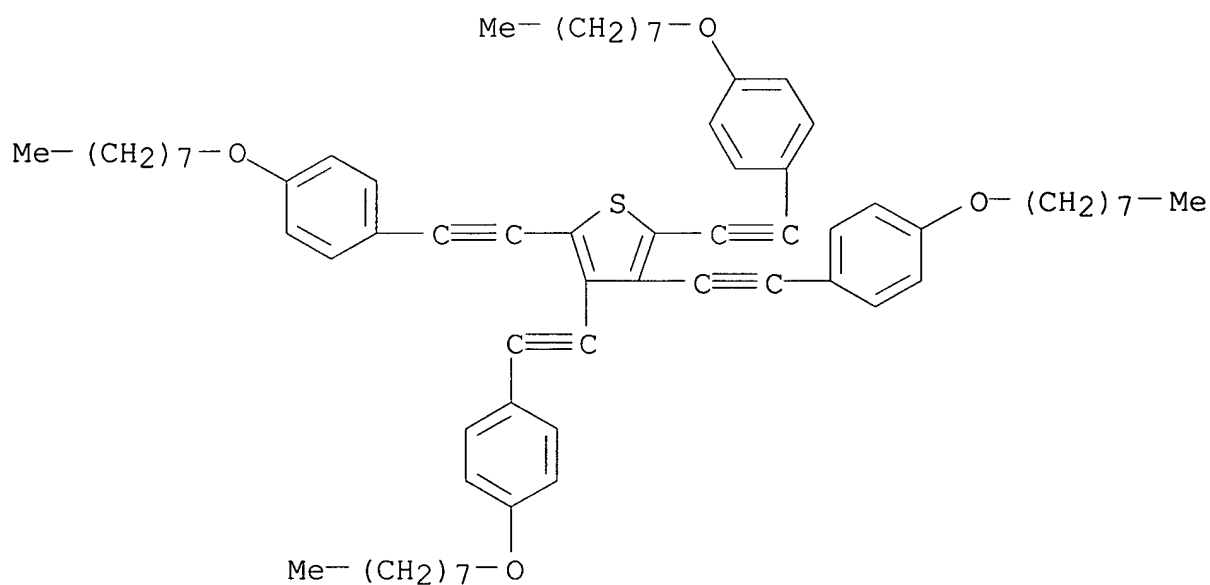
RN 727705-52-4 HCA

CN Thiophene, tetrakis[[4-(hexyloxy)phenyl]ethynyl]- (9CI) (CA INDEX NAME)



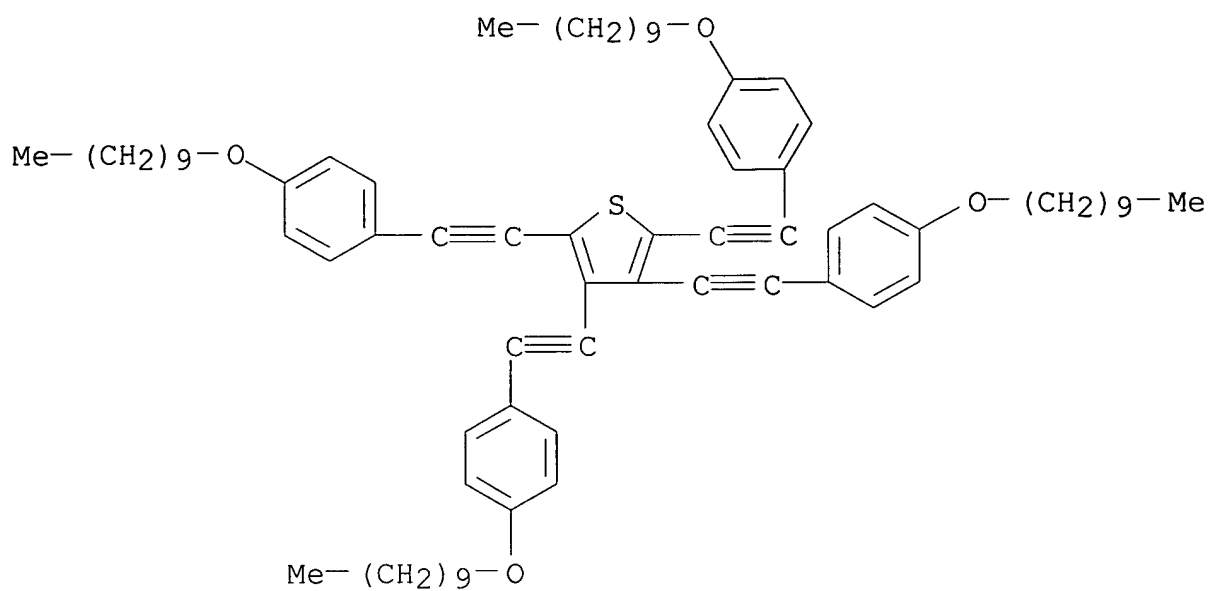
RN 727705-53-5 HCA

CN Thiophene, tetrakis[[4-(octyloxy)phenyl]ethynyl]- (9CI) (CA INDEX NAME)



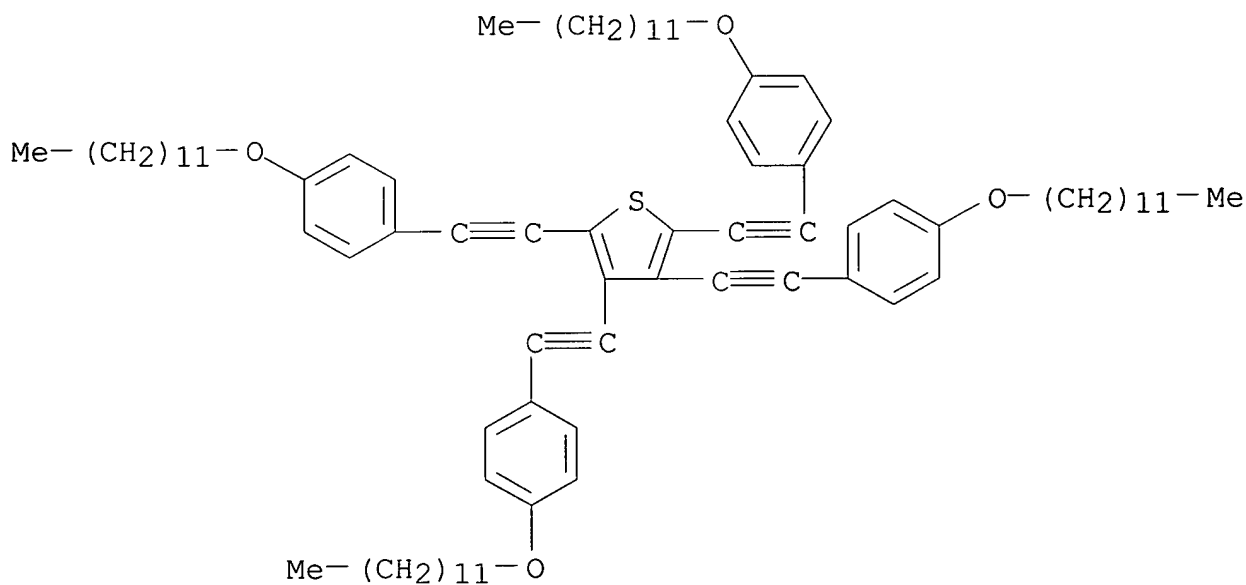
RN 727705-54-6 HCA

CN Thiophene, tetrakis[[4-(decyloxy)phenyl]ethynyl]- (9CI) (CA INDEX NAME)



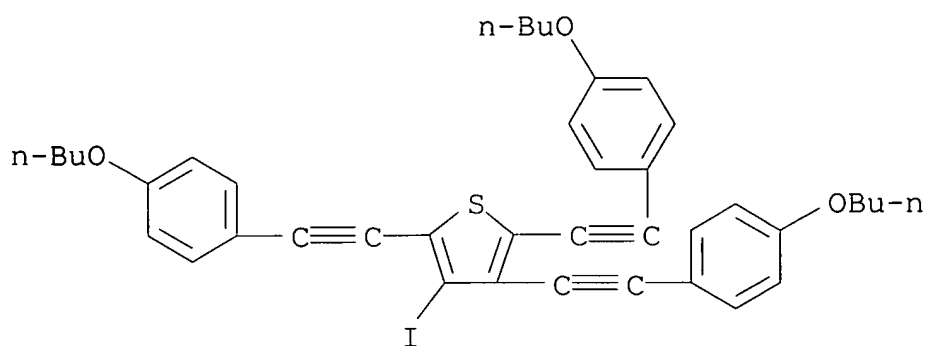
RN 727705-55-7 HCA

CN Thiophene, tetrakis[[4-(dodecyloxy)phenyl]ethynyl]- (9CI) (CA INDEX NAME)

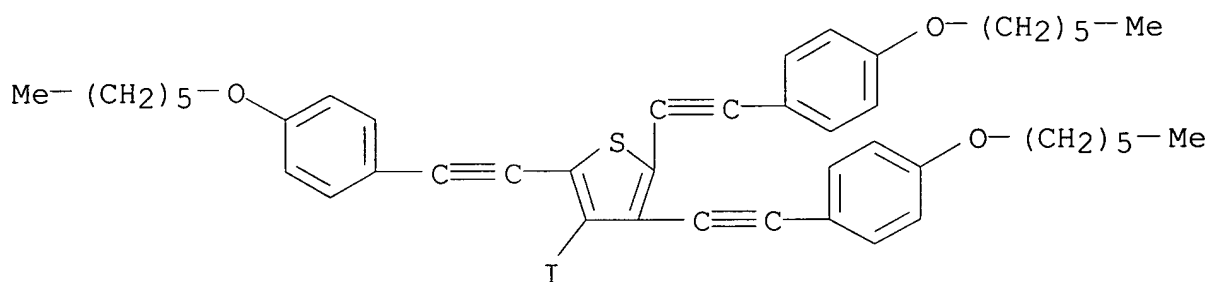


RN 727705-56-8 HCA

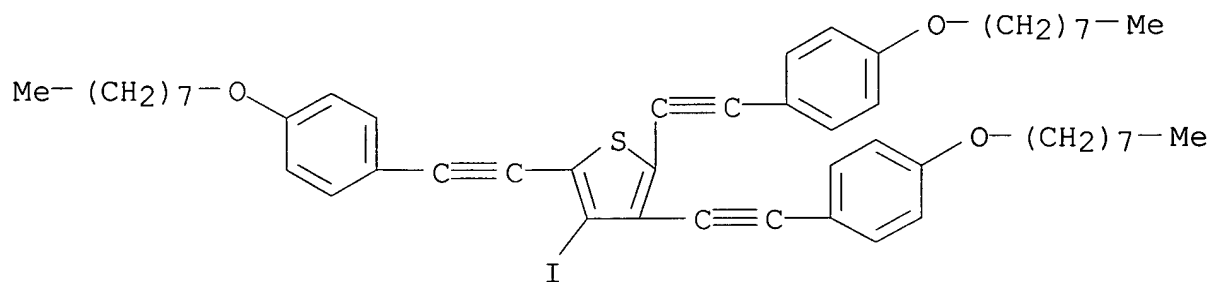
CN Thiophene, 2,3,5-tris[(4-butoxyphenyl)ethynyl]-4-iodo- (9CI) (CA INDEX NAME)



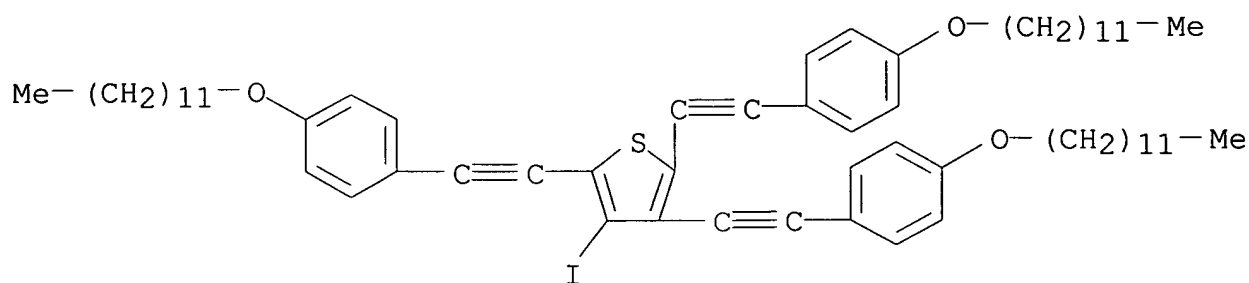
RN 727705-57-9 HCA
 CN Thiophene, 2,3,5-tris[[4-(hexyloxy)phenyl]ethynyl]-4-iodo- (9CI)
 (CA INDEX NAME)



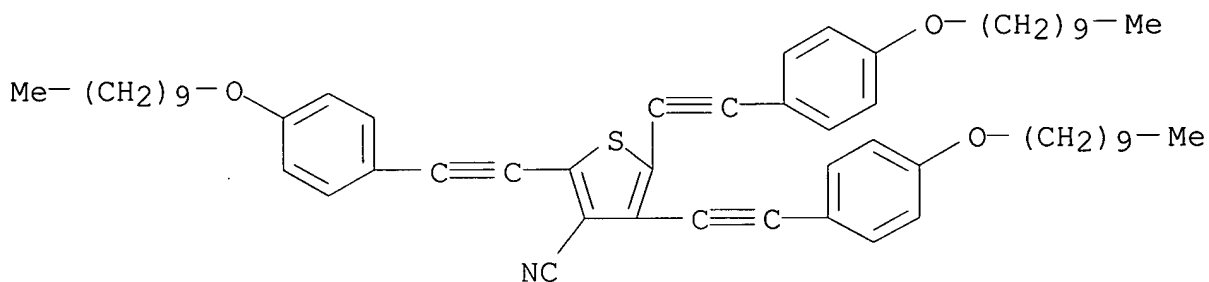
RN 727705-58-0 HCA
 CN Thiophene, 3-iodo-2,4,5-tris[[4-(octyloxy)phenyl]ethynyl]- (9CI)
 (CA INDEX NAME)



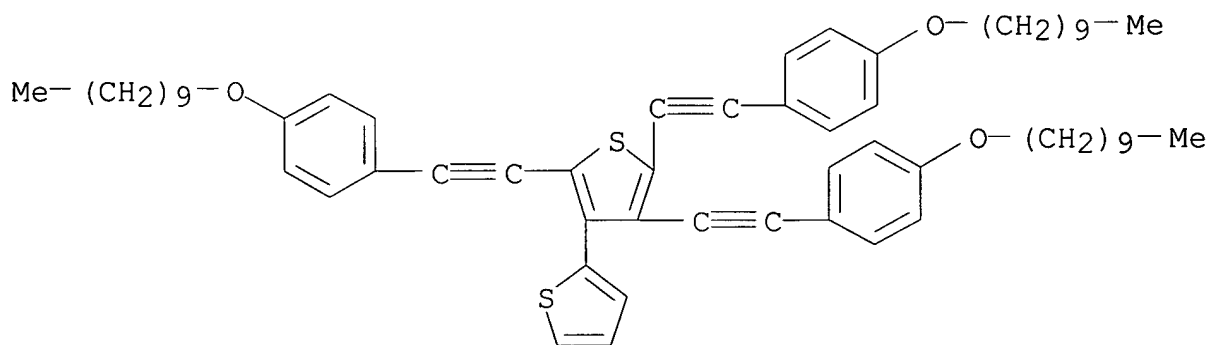
RN 727705-60-4 HCA
 CN Thiophene, 2,3,5-tris[[4-(dodecyloxy)phenyl]ethynyl]-4-iodo- (9CI)
 (CA INDEX NAME)



RN 727705-61-5 HCA
 CN 3-Thiophenecarbonitrile, 2,4,5-tris[[4-(decyloxy)phenyl]ethynyl]-
 (9CI) (CA INDEX NAME)



RN 727705-62-6 HCA
 CN 2,3'-Bithiophene, 2',4',5'-tris[[4-(decyloxy)phenyl]ethynyl]- (9CI)
 (CA INDEX NAME)

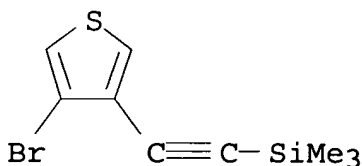


CC 27-8 (Heterocyclic Compounds (One Hetero Atom))
 Section cross-reference(s): 22, 69, 75

IT **Liquid crystals**
 (nematic; prepn., mol. geometry and thermal and mesomorphic
 properties of poly(alkoxyphenylethynyl)thiophenes)

IT **727705-59-1P**
 (prepn., mol. geometry and thermal and mesomorphic properties of

- poly(alkoxyphenylethynyl)thiophenes)
- IT 727705-51-3P 727705-52-4P 727705-53-5P
727705-54-6P 727705-55-7P 727705-56-8P
727705-57-9P 727705-58-0P 727705-60-4P
727705-61-5P 727705-62-6P
(prepn., mol. geometry and thermal and mesomorphic properties of
poly(alkoxyphenylethynyl)thiophenes)
- L40 ANSWER 4 OF 18 HCA COPYRIGHT 2005 ACS on STN
- 140:321944 Production of polymeric compositions comprising
thieno[3,4-b]thiophene. Sotzing, Gregory Allen (USA). U.S. Pat.
Appl. Publ. US 2004074779 A1 20040422, 8 pp. (English). CODEN:
USXXCO. APPLICATION: US 2003-618262 20030711. PRIORITY: US
2002-PV395183 20020711.
- AB A process comprises electrochem. reaction of a monomeric compn.
comprising thieno[3,4-b]thiophene, to form a polymeric compn.
comprising units derived from thieno[3,4-b]thiophene. Water-borne
dispersions of such polymers and copolymers can be cast by
conventional methods to provide uniform, thin films which possess
utility in numerous electroactive applications including
electrochromic displays, optically transparent electrodes and
antistatic coatings. Thus, thieno[3,4-b]thiophene was
prepd. from 3-bromo-4-(trimethylsilyl)ethynylthiophene, and polymd.
using ammonium persulfate and iron persulfate as oxidants to give
polythieno[3,4-b]thiophene.
- IT 131390-83-5, 3-Bromo-4-(trimethylsilyl)ethynyl-thiophene
(starting materials; polymeric compns. comprising
thieno[3,4-b]thiophene, method of making, and use thereof)
- RN 131390-83-5 HCA
- CN Silane, [(4-bromo-3-thienyl)ethynyl]trimethyl- (9CI) (CA INDEX
NAME)



- IC ICM C08G075-00
ICS C08G075-32; C25B003-00
- INCL 205414000; 528377000
- CC 35-7 (Chemistry of Synthetic High Polymers)
Section cross-reference(s): 74
- ST polythienothiophene electrochromic display transparent electrode
antistatic coating
- IT Coating materials
(**antistatic**; polymeric compns. comprising

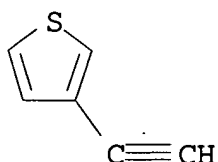
- thieno[3,4-b]thiophene, method of making, and use thereof)
- IT **Conducting polymers**
(polythiophenes; polymeric compns. comprising
thieno[3,4-b]thiophene, method of making, and use thereof)
- IT **131390-83-5**, 3-Bromo-4-(trimethylsilyl)ethynyl-thiophene
(starting materials; polymeric compns. comprising
thieno[3,4-b]thiophene, method of making, and use thereof)

L40 ANSWER 5 OF 18 HCA COPYRIGHT 2005 ACS on STN

140:254090 Monomeric, oligomeric and polymeric 3-alkynylthiophenes
useful as **charge transport** materials. Heeney,
Martin; Tierney, Steven; Bailey, Clare; McCulloch, Iain (Merck
Patent G.m.b.H., Germany). Eur. Pat. Appl. EP 1398336 A1 20040317,
26 pp. DESIGNATED STATES: R: AT, BE, CH, DE, DK, ES, FR, GB, GR,
IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR,
BG, CZ, EE, HU, SK. (English). CODEN: EPXXDW. APPLICATION: EP
2003-18346 20030813. PRIORITY: EP 2002-20711 20020914.

AB The invention relates to monomers, oligomers and polymers of the
general formula [(A)a-(B)b-(C)c-(D)d]_n (I), where A and C are
independently 2,5-thiophene units substituted with -C.tplbond.C-R1
and -R2 in 3 and 4 positions, resp.; R1 is in each occurrence
independently H, halogen, linear, branched or cyclic C1-C20-alkyl,
which is unsubstituted, monosubstituted or polysubstituted with F,
Cl, Br, I or CN, with one or more nonadjacent CH2 groups being
optionally and independently replaced with -O-, -S-, -NH-, -NR4-,
-SiR4R5-, -CO-, -COO-, -OCO-, -OCO-O-, -SO2-, -S-CO-, -CO-S-,
-CH=CH- or -C.tplbond.C-, the O and/or S atoms being not linked
directly to one another, or R1 denotes optionally substituted aryl,
heteroaryl, or P-Sp-X unit; R2 has one of the meanings of R1 or
denotes -C.tplbond.C-R3 group, the recurring units
[(A)a-(B)b-(C)c-(D)d] being identical or different. In the formula
(I), R3 has one of the meanings of R1; R4 and R5 are independently H
or C1-C12-alkyl; P is a polymerizable or reactive group; Sp is a
spacer group or a single bond; B and D are independently -CX1=CX2-,
-C.tplbond.C-, or optionally substituted arylene or heteroarylene;
X1 and X2 are independently H, F, Cl or CN; a, b, c, d are
independently 0 or 1, with (a+b+c+d) > 0, at least one of a and c
being 1 in at least one recurring unit [(A)a-(B)b-(C)c-(D)d]; and n
is an integer .gtoreq. 1. The monomeric, oligomeric and polymeric
3-alkynylthiophenes of the invention can be used as semiconductors
or **charge transport** materials in optical,
electrooptical or electronic devices, such as components of
integrated circuits, **field effect**
transistors for flat panel displays or radio frequency
identification tags, **electroluminescent** displays, liq.
crystal displays, photovoltaic or sensor devices, as electrode
materials in batteries, as photoconductors, and for
electrophotog. applications.

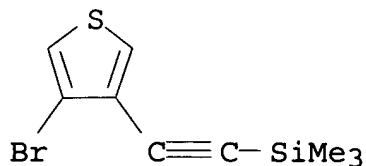
IT 67237-53-0DP, 3-Ethynylthiophene, derivs.
 (monomeric, oligomeric and polymeric 3-alkynylthiophenes useful
 as **charge transport** materials)
 RN 67237-53-0 HCA
 CN Thiophene, 3-ethynyl- (9CI) (CA INDEX NAME)



IC ICM C08G061-12
 CC 35-7 (Chemistry of Synthetic High Polymers)
 Section cross-reference(s): 27, 75, 76
 ST alkynylthiophene monomer oligomer polymer **charge transport** material elec device
 IT **Electric conductors**
 (anisotropic film; monomeric, oligomeric and polymeric
 3-alkynylthiophenes useful as **charge transport**
 materials)
 IT **Electroluminescent devices**
 (displays; monomeric, oligomeric and polymeric
 3-alkynylthiophenes useful as **charge transport**
 materials)
 IT Films
 (elec. conductive, anisotropic; monomeric, oligomeric and
 polymeric 3-alkynylthiophenes useful as **charge transport**
 materials)
 IT **Anisotropic materials**
 (elec. conductors, films; monomeric, oligomeric and polymeric
 3-alkynylthiophenes useful as **charge transport**
 materials)
 IT **Luminescent screens**
 (electroluminescent; monomeric, oligomeric and
 polymeric 3-alkynylthiophenes useful as **charge transport**
 materials)
 IT **Antistatic materials**
 (films; monomeric, oligomeric and polymeric 3-alkynylthiophenes
 useful as **charge transport** materials)
 IT **Optical imaging devices**
 (flat panels; monomeric, oligomeric and polymeric
 3-alkynylthiophenes useful as **charge transport**
 materials)
 IT **Electric conductors**
 Electrodes
 Electroluminescent devices

- Electrophotographic apparatus
- Field effect transistors
- Integrated circuits
- Liquid crystal displays
- Liquid crystals
- Photoconductors
- Photoelectric devices
- Safety devices
- Semiconductor materials
- Sensors
- Thin film transistors
 - (monomeric, oligomeric and polymeric 3-alkynylthiophenes useful as **charge transport** materials)
- IT Polyacetylenes, preparation
 - (polythiophene-; monomeric, oligomeric and polymeric 3-alkynylthiophenes useful as **charge transport** materials)
- IT **Conducting polymers**
 - (polythiophenes; monomeric, oligomeric and polymeric 3-alkynylthiophenes useful as **charge transport** materials)
- IT 67237-53-0DP, 3-Ethynylthiophene, derivs.
 - (monomeric, oligomeric and polymeric 3-alkynylthiophenes useful as **charge transport** materials)
- L40 ANSWER 6 OF 18 HCA COPYRIGHT 2005 ACS on STN
- 140:77587 Polymers comprising thieno[3,4-b]thiophene and methods of making and using the same. Sotzing, Gregory Allen (USA). U.S. Pat. Appl. Publ. US 2004010115 A1 20040115, 9 pp. (English). CODEN: USXXCO. APPLICATION: US 2002-193598 20020711.
- AB This invention presents polymers and copolymers comprising repeating units of thieno[3,4-b]thiophene. Water-borne dispersions of such polymers and copolymers can be cast by conventional methods to provide uniform, thin films which possess utility in numerous electroactive applications including electrochromic displays, optically transparent electrodes and **antistatic** coatings. The compns. of this invention can be doped with conventional p-dopants or n-dopants. The invention also presents an aq. process for prepg. such compns. of matter. Thus, thieno[3,4-b]thiophene was prepd. from 3-bromo-4-(trimethylsilyl)ethynylthiophene, and polymd. using ammonium persulfate and iron persulfate as oxidants to give polythieno[3,4-b]thiophene.
- IT 131390-83-5, 3-Bromo-4-(trimethylsilyl)ethynylthiophene
 - (starting materials; prodn. of thieno[3,4-b]thiophene polymers for electrochromic displays, transparent electrodes, and **antistatic** coatings)
- RN 131390-83-5 HCA
- CN Silane, [(4-bromo-3-thienyl)ethynyl]trimethyl- (9CI) (CA INDEX

NAME)



- IC ICM C08G075-00
- INCL 528377000
- CC 35-7 (Chemistry of Synthetic High Polymers)
Section cross-reference(s): 42, 74
- ST polythienothiophene electrochromic display transparent electrode
antistatic coating
- IT Coating materials
(**antistatic**; prodn. of thieno[3,4-b]thiophene polymers
for electrochromic displays, transparent electrodes, and
antistatic coatings)
- IT Polymerization
(electrochem.; prodn. of thieno[3,4-b]thiophene polymers for
electrochromic displays, transparent electrodes, and
antistatic coatings)
- IT Polymerization
(oxidative; prodn. of thieno[3,4-b]thiophene polymers for
electrochromic displays, transparent electrodes, and
antistatic coatings)
- IT **Conducting polymers**
(polythiophenes; prodn. of thieno[3,4-b]thiophene polymers for
electrochromic displays, transparent electrodes, and
antistatic coatings)
- IT Electrochromic imaging devices
Oxidizing agents
Transparent films
(prodn. of thieno[3,4-b]thiophene polymers for electrochromic
displays, transparent electrodes, and **antistatic**
coatings)
- IT Electrodes
(transparent; prodn. of thieno[3,4-b]thiophene polymers for
electrochromic displays, transparent electrodes, and
antistatic coatings)
- IT 250-65-7P, Thieno[3,4-b]thiophene
(monomer; prodn. of thieno[3,4-b]thiophene polymers for
electrochromic displays, transparent electrodes, and
antistatic coatings)
- IT 7553-56-2, Iodine, uses 7705-08-0, Iron trichloride, uses
7722-64-7, Potassium permanganate 7722-84-1, Hydrogenperoxide,
uses 7727-54-0, Ammonium persulfate 7778-50-9, Potassium

dichromate 7782-44-7, Oxygen, uses 10028-22-5, Diiron trisulfate 13537-24-1, Iron triperchlorate 38465-60-0, Copper tetrafluoroborate

(oxidant; prodn. of thieno[3,4-b]thiophene polymers for electrochromic displays, transparent electrodes, and **antistatic** coatings)

IT 9003-01-4, Polyacrylic acid 25087-26-7, Polymethacrylic acid 26099-09-2, Polymaleic acid 26101-52-0, Polyvinyl sulfonic acid 50851-57-5, Polystyrene sulfonic acid

(polyanion; prodn. of thieno[3,4-b]thiophene polymers for electrochromic displays, transparent electrodes, and **antistatic** coatings)

IT 109-72-8, n-Butyl lithium, uses

(prodn. of thieno[3,4-b]thiophene polymers for electrochromic displays, transparent electrodes, and **antistatic** coatings)

IT 142189-51-3P, Polythieno[3,4-b]thiophene 425621-50-7P, 3,4-Ethylenedioxythiophenethieno[3,4-b]thiophene copolymer 425927-19-1P, 3-Octylthiophene-thieno[3,4-b]thiophene copolymer (prodn. of thieno[3,4-b]thiophene polymers for electrochromic displays, transparent electrodes, and **antistatic** coatings)

IT 1923-70-2, Tetrabutylammonium perchlorate 3109-63-5, Tetrabutylammonium hexafluorophosphate

(prodn. of thieno[3,4-b]thiophene polymers for electrochromic displays, transparent electrodes, and **antistatic** coatings)

IT 131390-83-5, 3-Bromo-4-(trimethylsilyl)ethynylthiophene (starting materials; prodn. of thieno[3,4-b]thiophene polymers for electrochromic displays, transparent electrodes, and **antistatic** coatings)

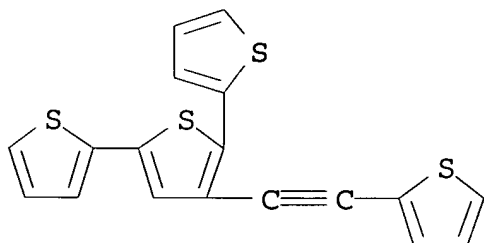
L40 ANSWER 7 OF 18 HCA COPYRIGHT 2005 ACS on STN

138:255614 Polyterthiophene Appended by Organomolybdenum Sulfide Cluster: Electrochemical Synthesis and Electrochemical Properties of Poly[Mo₂(.mu.-C₅H₅)₂{.mu.-.eta.²:.eta.²-SC(R):C S[C₄HS(C₄H₃S-2)₂-2,5]}₂]s. Kim, Dong Hyun; Kim, Joo-Hwan; Kim, Tae Ho; Kang, Dong Min; Kim, Yong Hwan; Shim, Yoon-Bo; Shin, Sung Chul (Department of Chemistry, Gyeongsang National University, Jinju, 660-701, S. Korea). Chemistry of Materials, 15(4), 825-827 (English) 2003. CODEN: CMATEX. ISSN: 0897-4756. Publisher: American Chemical Society.

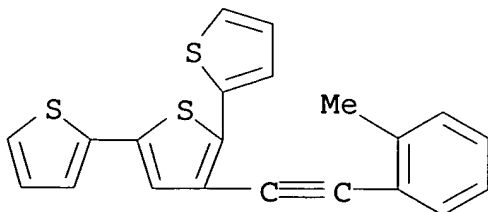
AB Polythiophene hybrids were synthesized by electrochem. polymn. of monomer clusters of formula [(CpMo)₂(SC(R):CS[C₄HS(C₄H₃S-2)₂-2,5]]₂]s, where R = H, Ph, Bu, thienyl, tolyl. The monomer clusters were prep'd. by the reaction of 3'-(alkynyl)-2,2':5',2''-terthiophenes with (CpMo)₂(SC₃H₆S)₂ in CH₂Cl₂ and isolated as reddish brown solids by column chromatog. in 15-46 % yield. The

crystal structure of the clusters was elucidated; e.g., the at. connection of the phenyl-cluster has a syn isomer in terthienyl/terthienyl orientation around Mo. Cyclic voltammograms (CV) of the clusters in CH₂Cl₂ contg. 0.1 M tetrabutylammonium phosphate (TBAP) show chem. reversibility for generation of the Mo⁺ and Mo²⁺ species and an irreversible wave at 1.30 - 1.41 V assigned to oxidn. of terthienyl moiety, i.e., electrochem. polymn. Polythiophene clusters were prepd. by potential cycling on Pt disk electrodes or ITO coated glass electrodes in CH₂Cl₂ contg. 0.1 M TBAP at 0.0 to 1.5 V and scan rate 100 mV s⁻¹. The polythiophene clusters show color switching between brown (neutral) and gray (oxidized) states, a unique electrochromism distinguishable from that of thiophene-based conducting polymers. Such unique electrochromism is attributed to electronic synergistic interactions between Mo sulfide cluster units and the polythiophene .pi.-backbone.

IT 502962-87-0P, 3'-(2-Thienylethynyl)-2,2':5',2''-terthiophene
 502962-88-1P, 3'-(o-Tolyethynyl)-2,2':5',2''-terthiophene
 (intermediate; prepn. of terthiophene molybdenum sulfide cluster monomers and electrooxidative polymn. producing conducting electrochromic polythiophenes)
 RN 502962-87-0 HCA
 CN 2,2':5',2''-Terthiophene, 3'-(2-thienylethynyl)- (9CI) (CA INDEX NAME)



RN 502962-88-1 HCA
 CN 2,2':5',2''-Terthiophene, 3'-[(2-methylphenyl)ethynyl]- (9CI) (CA INDEX NAME)

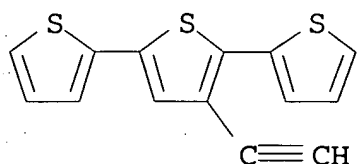


IT 208125-85-3, 3'-(Ethynyl)-2,2':5',2''-terthiophene

(prepn. of terthiophene molybdenum sulfide cluster monomers and electrooxidative polymn. producing conducting electrochromic polythiophenes)

RN 208125-85-3 HCA

CN 2,2':5',2''-Terthiophene, 3'-ethynyl- (9CI) (CA INDEX NAME)



CC 35-7 (Chemistry of Synthetic High Polymers)
Section cross-reference(s): 29, 36, 72, 75, 76

IT **Conducting polymers**
(polythiophenes, polyterthiophene-Mo cluster; prepn. of terthiophene molybdenum sulfide cluster monomers and electrooxidative polymn. producing conducting electrochromic polythiophenes)

IT **Conducting polymers**
Crystal structure
Electrochromism
Molecular orientation
Molecular structure
Oxidation, electrochemical
Redox potential
(prepn. of terthiophene molybdenum sulfide cluster monomers and electrooxidative polymn. producing conducting electrochromic polythiophenes)

IT 502962-86-9P 502962-87-0P, 3'-(2-Thienylethynyl)-2,2':5',2''-terthiophene 502962-88-1P, 3'-(o-Tolyethynyl)-2,2':5',2''-terthiophene
(intermediate; prepn. of terthiophene molybdenum sulfide cluster monomers and electrooxidative polymn. producing conducting electrochromic polythiophenes)

IT 106-38-7, 4-Bromotoluene 693-02-7, 1-Hexyne 1003-09-4, 2-Bromothiophene 72186-30-2 105125-00-6, 3'-Bromo-2,2':5',2''-terthiophene 208125-85-3, 3'-(Ethynyl)-2,2':5',2''-terthiophene
(prepn. of terthiophene molybdenum sulfide cluster monomers and electrooxidative polymn. producing conducting electrochromic polythiophenes)

L40 ANSWER 8 OF 18 HCA COPYRIGHT 2005 ACS on STN

137:279707 Poly(thieno[3,4-b]thiophene): A p- and n-Dopable Polythiophene Exhibiting High Optical Transparency in the Semiconducting State. Sotzing, Gregory A.; Lee, Kyunghoon

(Department of Chemistry and the Polymer Program, Institute of Materials Science, University of Connecticut, Storrs, CT, 06269-3136, USA). Macromolecules, 35(19), 7281-7286 (English) 2002. CODEN: MAMOBX. ISSN: 0024-9297. Publisher: American Chemical Society.

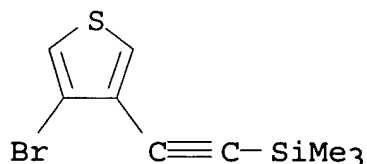
AB Herein we report the synthesis and electrochem. characterization of poly(thieno[3,4-b]thiophene) (Poly(T34bT)), a new low band gap conducting polymer with a high redox switching stability that exhibits high optical transparency in the semiconductive state. The monomer, thieno[3,4-b]thiophene (T34bT), has a low oxidn. potential for polymn., 1.02 V vs. Ag/Ag⁺ (1.25 V vs. SCE), a potential between that for the oxidn. of 3,4-ethylenedioxythiophene and pyrrole. Poly(T34bT) has a band gap of ca. 0.85 eV (1459 nm) as detd. by the onset for the .pi.-to-.pi.* transition from the UV-vis-NIR spectrum and 0.8 V from the difference in the onsets for both the p- and n-doping processes from cyclic voltammetry. Stability studies as detd. from chronocoulometry and chronoabsorptometry indicate that the polymer retains 95% electroactivity and 96% change in optical d. after 100 double potential steps. Poly(T34bT) is sky-blue in the reduced form and optically transparent (no observable color) in the oxidized state with a coloration efficiency of 160 cm²/C at 800 nm.

IT 131390-83-5

(initial reagent for synthesis of thieno[3,4-b]thiophene)

RN 131390-83-5 HCA

CN Silane, [(4-bromo-3-thienyl)ethynyl]trimethyl- (9CI) (CA INDEX NAME)



CC 36-5 (Physical Properties of Synthetic High Polymers)
Section cross-reference(s): 28, 72

IT **Conducting polymers**

(synthesis of electrochem. characterization of
poly(thieno[3,4-b]thiophene))

IT 131390-83-5

(initial reagent for synthesis of thieno[3,4-b]thiophene)

L40 ANSWER 9 OF 18 HCA COPYRIGHT 2005 ACS on STN

135:358490 Synthesis of poly(thieno[3,4-b]thiophene) and its electrochemical characterization. Lee, Kyunghoon; Sotzing, Gregory A. (Department of Chemistry and the Polymer Program, Institute of Materials Science, University of Connecticut, Storrs, CT, 06269, USA). Polymer Preprints (American Chemical Society, Division of

Polymer Chemistry), 42(2), 413-414 (English) 2001. CODEN: ACPPAY.
ISSN: 0032-3934. Publisher: American Chemical Society, Division of
Polymer Chemistry.

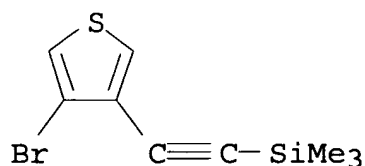
AB Synthesis of poly(thieno[3,4-b]thiophene) and its electrochem.
characterization is carried out.

IT 131390-83-5

(initial reagent for synthesis of thieno[3,4-b]thiophene)

RN 131390-83-5 HCA

CN Silane, [(4-bromo-3-thienyl)ethynyl]trimethyl- (9CI) (CA INDEX
NAME)



CC 37-2 (Plastics Manufacture and Processing)
Section cross-reference(s): 23, 72

IT **Conducting polymers**

(synthesis of electrochem. characterization of
poly(thieno[3,4-b]thiophene))

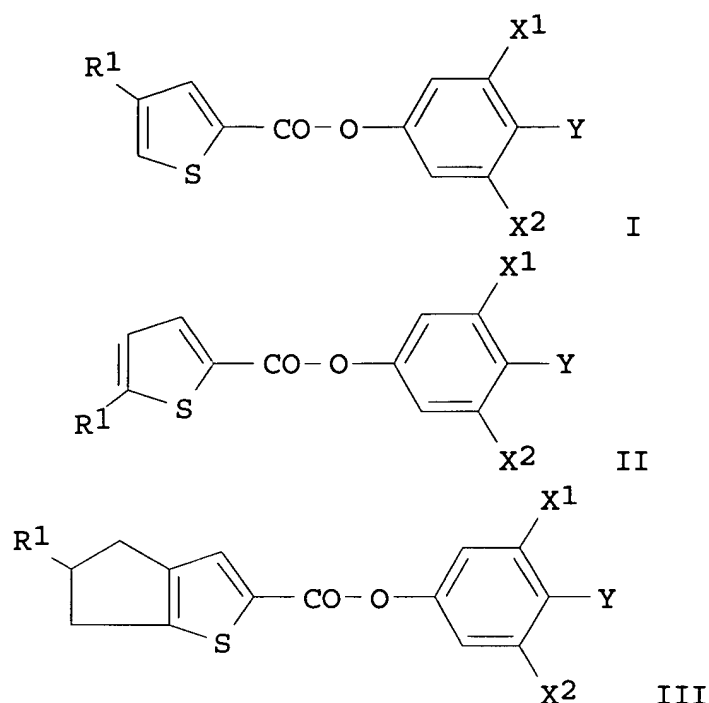
IT 131390-83-5

(initial reagent for synthesis of thieno[3,4-b]thiophene)

L40 ANSWER 10 OF 18 HCA COPYRIGHT 2005 ACS on STN

135:203104 Thiophene carboxylic acid ester and liquid crystalline medium
suitable for liquid crystal display. Reiffenrath, Volker;
Hirschmann, Harald (Merck Patent G.m.b.H., Germany). Ger. Offen. DE
10102631 A1 20010830, 18 pp. (German). CODEN: GWXXBX.
APPLICATION: DE 2001-10102631 20010120. PRIORITY: DE 2000-10009234
20000228.

GI



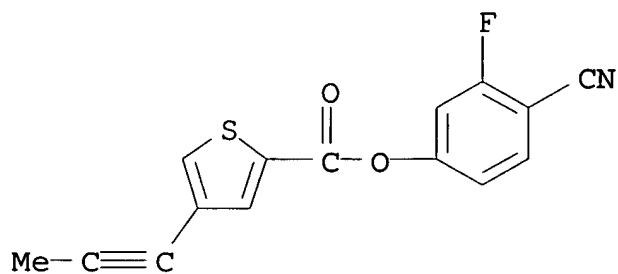
AB The new thiophene carboxylic acid ester is represented by I, II, or III ($R_1 = H, C_{1-12}\text{-alkyl}$; $X_1, X_2 = H, F$; $Y = CN, F, OCF_3, OCHF_2, CF_3, OC_2F_5, \text{perfluoroalkyl}$) and synthesized. The liq. cryst. medium comprises at least 2 liq. cryst. components in which at least one compd. is the above thiophene carboxylic acid ester. The liq. cryst. medium is suitable for a liq. crystal display.

IT 356063-99-5P 356064-00-1P 356064-01-2P
 356064-02-3P 356064-03-4P 356064-24-9P
 356064-25-0P 356064-26-1P 356064-27-2P
 356064-28-3P

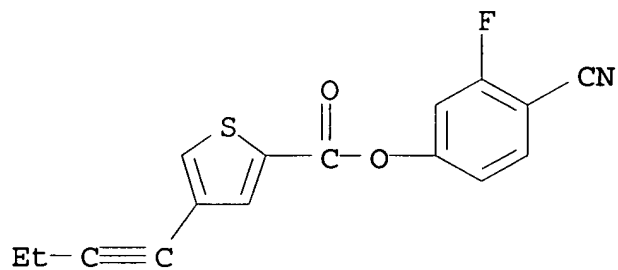
(synthesis of new thiophene carboxylic acid ester for liq. crystal mixt. suitable for liq. crystal display)

RN 356063-99-5 HCA

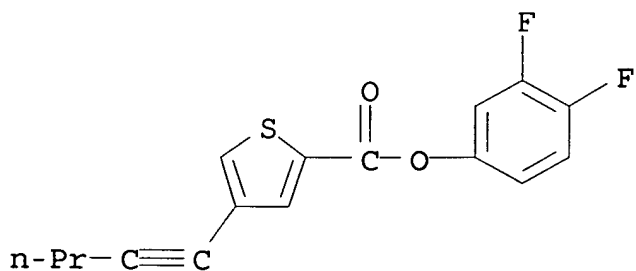
CN 2-Thiophenecarboxylic acid, 4-(1-propynyl)-, 4-cyano-3-fluorophenyl ester (9CI) (CA INDEX NAME)



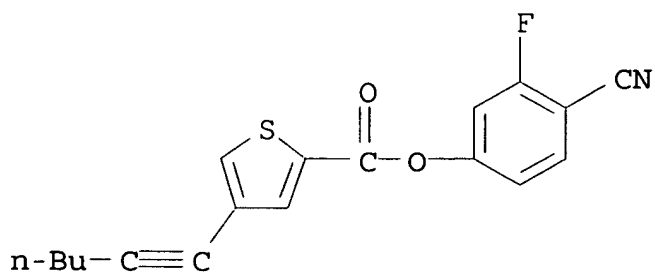
RN 356064-00-1 HCA
 CN 2-Thiophenecarboxylic acid, 4-(1-butynyl)-, 4-cyano-3-fluorophenyl ester (9CI) (CA INDEX NAME)



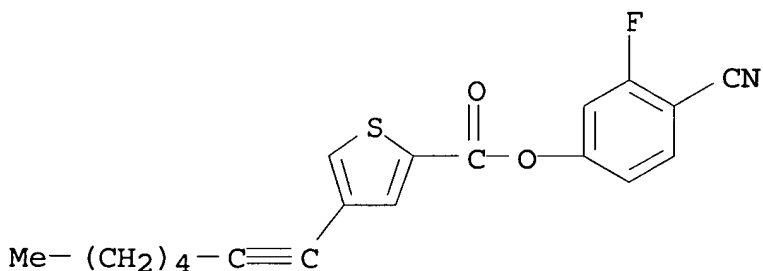
RN 356064-01-2 HCA
 CN 2-Thiophenecarboxylic acid, 4-(1-pentynyl)-, 3,4-difluorophenyl ester (9CI) (CA INDEX NAME)



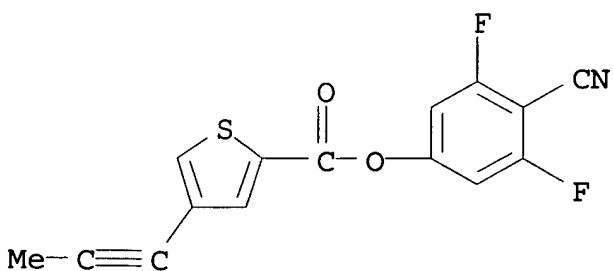
RN 356064-02-3 HCA
 CN 2-Thiophenecarboxylic acid, 4-(1-hexynyl)-, 4-cyano-3-fluorophenyl ester (9CI) (CA INDEX NAME)



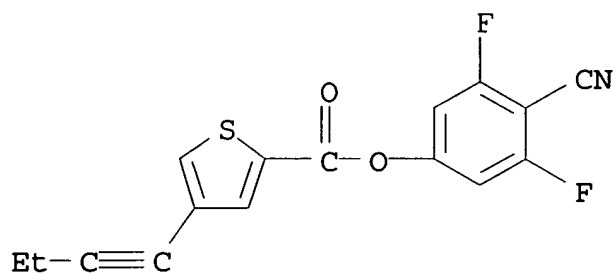
RN 356064-03-4 HCA
 CN 2-Thiophenecarboxylic acid, 4-(1-heptynyl)-, 4-cyano-3-fluorophenyl ester (9CI) (CA INDEX NAME)



RN 356064-24-9 HCA
 CN 2-Thiophenecarboxylic acid, 4-(1-propynyl)-, 4-cyano-3,5-difluorophenyl ester (9CI) (CA INDEX NAME)

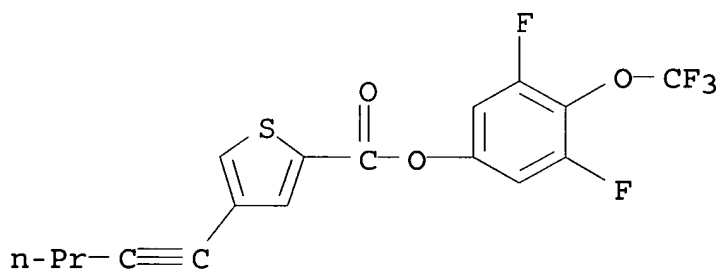


RN 356064-25-0 HCA
 CN 2-Thiophenecarboxylic acid, 4-(1-butynyl)-, 4-cyano-3,5-difluorophenyl ester (9CI) (CA INDEX NAME)



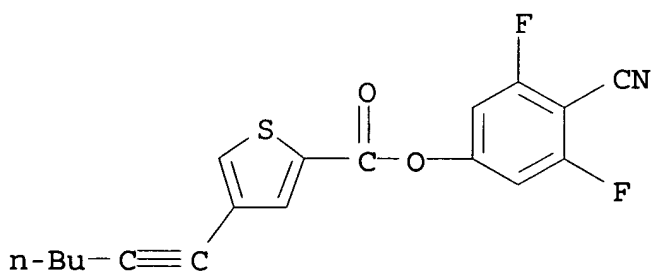
RN 356064-26-1 HCA

CN 2-Thiophenecarboxylic acid, 4-(1-pentynyl)-, 3,5-difluoro-4-(trifluoromethoxy)phenyl ester (9CI) (CA INDEX NAME)



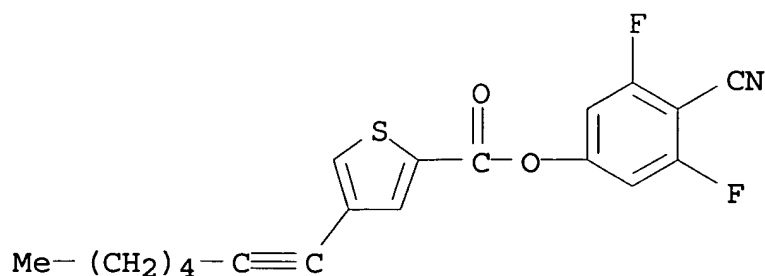
RN 356064-27-2 HCA

CN 2-Thiophenecarboxylic acid, 4-(1-hexynyl)-, 4-cyano-3,5-difluorophenyl ester (9CI) (CA INDEX NAME)



RN 356064-28-3 HCA

CN 2-Thiophenecarboxylic acid, 4-(1-heptynyl)-, 4-cyano-3,5-difluorophenyl ester (9CI) (CA INDEX NAME)



- IC ICM C07D333-40
ICS C07D333-50; C09K019-34; G09F009-35
- CC 74-13 (Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes)
Section cross-reference(s): 75
- IT **Liquid crystals**
(nematic; synthesis of new thiophene carboxylic acid ester for liq. crystal mixt. suitable for liq. crystal display)
- IT **Liquid crystal displays**
(synthesis of new thiophene carboxylic acid ester for liq. crystal mixt. suitable for liq. crystal display)
- IT 120917-49-9P 120917-50-2P 356063-89-3P 356063-90-6P
356063-91-7P 356063-92-8P 356063-93-9P 356063-94-0P
356063-95-1P 356063-96-2P 356063-97-3P 356063-98-4P
356063-99-5P 356064-00-1P 356064-01-2P
356064-02-3P 356064-03-4P 356064-04-5P
356064-05-6P 356064-06-7P 356064-07-8P 356064-08-9P
356064-09-0P 356064-10-3P 356064-11-4P 356064-12-5P
356064-13-6P 356064-14-7P 356064-15-8P 356064-16-9P
356064-17-0P 356064-18-1P 356064-19-2P 356064-20-5P
356064-21-6P 356064-22-7P 356064-23-8P **356064-24-9P**
356064-25-0P 356064-26-1P 356064-27-2P
356064-28-3P 356064-29-4P 356064-30-7P 356064-31-8P
356064-32-9P 356064-33-0P 356064-34-1P 356064-35-2P
356064-36-3P 356064-37-4P 356064-38-5P 356064-39-6P
356064-41-0P 356064-42-1P 356064-43-2P 356064-44-3P
356064-45-4P 356064-46-5P 356064-47-6P 356064-48-7P
356064-49-8P 356064-50-1P 356064-51-2P 356064-52-3P
356064-53-4P 356064-54-5P 356064-55-6P 356064-56-7P
356064-57-8P 356064-58-9P 356064-59-0P 356064-60-3P
356064-61-4P 356064-63-6P 356064-64-7P 356064-65-8P
356064-66-9P 356064-67-0P 356064-68-1P 356064-69-2P
356064-70-5P 356064-71-6P 356064-72-7P 356064-73-8P
356064-74-9P 356064-75-0P 356064-76-1P 356064-77-2P
356064-78-3P 356064-79-4P 356064-80-7P 356064-81-8P
356064-82-9P 356064-83-0P 356064-84-1P 356064-85-2P
356064-86-3P 356064-87-4P 356064-88-5P 356064-89-6P

356064-90-9P	356064-91-0P	356064-92-1P	356064-93-2P
356064-94-3P	356064-95-4P	356064-96-5P	356064-97-6P
356064-98-7P	356064-99-8P	356065-00-4P	356065-01-5P
356065-02-6P	356065-03-7P	356065-04-8P	356065-05-9P
356065-06-0P	356065-07-1P	356065-08-2P	356065-09-3P
356065-10-6P	356065-11-7P	356065-12-8P	356065-13-9P
356065-14-0P	356065-15-1P	356065-16-2P	356065-17-3P
356065-18-4P	356065-19-5P	356065-20-8P	356065-21-9P
356065-22-0P	356065-23-1P	356065-25-3P	356065-26-4P
356065-27-5P	356065-28-6P	356065-29-7P	356065-30-0P
356065-31-1P	356065-32-2P	356065-33-3P	356066-27-8P
356066-28-9P			

(synthesis of new thiophene carboxylic acid ester for liq. crystal mixt. suitable for liq. crystal display)

L40 ANSWER 11 OF 18 HCA COPYRIGHT 2005 ACS on STN

134:200306 Cyclooctatetraenes as **electron transporters**

in organic **light emitting** diodes. Weber,

William P.; Lu, Ping; Thompson, Mark E.; Hong, Haiping (The University of Southern California, USA). PCT Int. Appl. WO

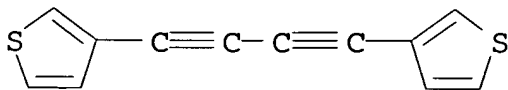
2001013683 A1 20010222, 54 pp. DESIGNATED STATES: W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 2000-US22425 20000816. PRIORITY: US 1999-375125 19990816.

AB Org. **light-emitting** devices are described which are provided with **electron transporting** layers comprising a cyclooctatetraene deriv. (esp. a tetraaryl-tetraarylethynyl-cyclooctatetraene).

IT **81294-14-6DP**, tetramer
(org. **electroluminescent** devices using cyclooctatetraene deriv. **electron transport** layers)

RN 81294-14-6 HCA

CN Thiophene, 3,3'-(1,3-butadiyne-1,4-diyl)bis- (9CI) (CA INDEX NAME)

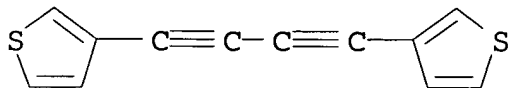


IT **81294-14-6**
(org. **electroluminescent** devices using

cyclooctatetraene deriv. **electron transport**
layers)

RN 81294-14-6 HCA

CN Thiophene, 3,3'-(1,3-butadiyne-1,4-diyl)bis- (9CI) (CA INDEX NAME)



IC ICM H05B033-12

CC 73-11 (Optical, Electron, and Mass Spectroscopy and Other Related Properties)

Section cross-reference(s): 25, 28, 76

ST tetraaryltetraarylethynyl cyclooctatetraene deriv **electron transport** layer **electroluminescent** device; org **electroluminescent** device cyclooctatetraene deriv **electron transport** layer

IT **Electron transport**

(org. **electroluminescent** devices using cyclooctatetraene deriv. **electron transport** layers)

IT **Electroluminescent** devices

(org.; org. **electroluminescent** devices using cyclooctatetraene deriv. **electron transport** layers)

IT 25360-32-1, Dihydridocarbonyltris(triphenylphosphine)ruthenium (org. **electroluminescent** devices using cyclooctatetraene deriv. **electron transport** layers)

IT 123847-85-8

(org. **electroluminescent** devices using cyclooctatetraene deriv. **electron transport** layers)

IT 198-55-0, Perylene

(org. **electroluminescent** devices using cyclooctatetraene deriv. **electron transport** layers)

IT 20199-36-4P **81294-14-6DP**, tetramer 151362-06-0DP, tetramer 294677-53-5P 294677-54-6P 294677-55-7P (org. **electroluminescent** devices using cyclooctatetraene deriv. **electron transport** layers)

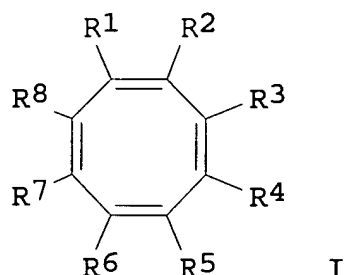
IT 886-66-8, Diphenylbutadiyne 20199-36-4D, tetramer 22779-05-1 **81294-14-6** 151362-06-0

(org. **electroluminescent** devices using cyclooctatetraene deriv. **electron transport** layers)

IT 22666-07-5P
(org. **electroluminescent** devices using
cyclooctatetraene deriv. **electron transport**
layers)

L40 ANSWER 12 OF 18 HCA COPYRIGHT 2005 ACS on STN
134:193144 Synthesis of cyclooctatetraene derivatives and their use as
electron transporters in organic light
emitting diodes. Weber, William P.; Lu, Ping; Thompson,
Mark E.; Hong, Haiping (The University of Southern California, USA).
PCT Int. Appl. WO 2001012576 A1 20010222, 57 pp. DESIGNATED
STATES: W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA,
CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM,
HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT,
LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD,
SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW,
AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH,
CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR,
NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2.
APPLICATION: WO 2000-US22428 20000816. PRIORITY: US 1999-375126
19990816.

GI

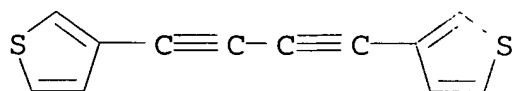


AB Cyclooctatetraene derivs. are described by the general formula I
(R1-8 = alkyl, aryl, and/or alkynyl groups; and .gtoreq.1 of R1-8 is
different from the other members of R1-8). Application as
electron transport materials in org.
electroluminescent devices is indicated.

IT **81294-14-6DP**, tetramer
(cyclooctatetraene derivs.)

RN 81294-14-6 HCA

CN Thiophene, 3,3'-(1,3-butadiyne-1,4-diyl)bis- (9CI) (CA INDEX NAME)

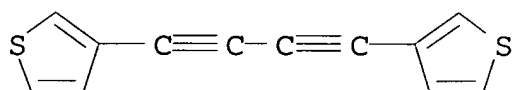


IT 81294-14-6

(cyclooctatetraene derivs.)

RN 81294-14-6 HCA

CN Thiophene, 3,3'-(1,3-butadiyne-1,4-diyl)bis- (9CI) (CA INDEX NAME)



IC ICM C07C015-12

CC 24-6 (Alicyclic Compounds)

Section cross-reference(s): 28, 73, 76

ST cyclooctatetraene deriv; org electroluminescent device

cyclooctatetraene deriv electron transport layer

IT **Electron transport**

(cyclooctatetraene derivs. as electron transport layers in org. electroluminescent devices)

IT **Electroluminescent devices**

(org.; cyclooctatetraene derivs. as electron transport layers in org. electroluminescent devices)

IT 20199-36-4DP, tetramer 81294-14-6DP, tetramer

151362-06-0DP, tetramer 294677-53-5P 294677-54-6P 294677-55-7P
(cyclooctatetraene derivs.)

IT 104-92-7, p-Bromoanisole 766-97-2, p-Tolylacetylene 886-66-8,

Diphenylbutadiyne 1066-54-2, Trimethylsilylacetylene 5929-72-6,

2,7-Dimethylocta-3,5-diyne-2,7-diol 20199-36-4 81294-14-6

151362-06-0

(cyclooctatetraene derivs.)

IT 198-55-0, Perylene 123847-85-8

(cyclooctatetraene derivs. as electron transport layers in org. electroluminescent devices)

L40 ANSWER 13 OF 18 HCA COPYRIGHT 2005 ACS on STN

132:50095 Synthesis of Tris(2,5-dialkynylthieno)cyclotriynes,

Tris(4,5-dialkoxyphenyl)cyclotriynes, and Tetrakis(4,5-dialkoxyphenyl)cyclotetraynes with Long-Chain Alkyl Substituents, and the Nickel and Cobalt Complexes of Tris[4,5-

(didecyloxy)phenyl]cyclotriyne. Zhang, Daming; Tessier, Claire A.;

Youngs, Wiley J. (Department of Chemistry, The University of Akron, Akron, OH, 44325-3601, USA). Chemistry of Materials, 11(11), 3050-3057 (English) 1999. CODEN: CMATEX. ISSN: 0897-4756. OTHER SOURCES: CASREACT 132:50095. Publisher: American Chemical Society.

AB This report focuses on the synthesis of materials designed to be discotic mesogens based on a cyclotriyne core with alkyl side chain substituents. With the attachment of long side chains, tris(4,5-dialkoxyphenyl)cyclotriynes and tris(2,5-dialkynylthieno)cyclotriynes are structurally similar to hexa-substituted triphenylene discotic mesophases. The syntheses of four tris(2,5-dialkynylthieno)cyclotriynes, two tris(4,5-dialkoxyphenyl)cyclotriynes, and two tetrakis(4,5-dialkoxyphenyl)cyclotetraynes are described. The structure of tris(2,5-dioctynylthieno)cyclotriyne was detd. by x-ray crystallog. (space group P63/m, Z = 2, wR(F) = 0.20); although the structure could not be solved completely, it was adequate to detn. the crystal packing. The interaction of one of the tris(4,5-dialkoxyphenyl)cyclotriynes with Ni(0) and Co₂(CO)₈ to form a mononuclear Ni(0) complex and a tetranuclear Co cluster are reported. Evidence is also presented to explain why the systems reported herein are not liq. crystals and suggestions for correcting this are made.

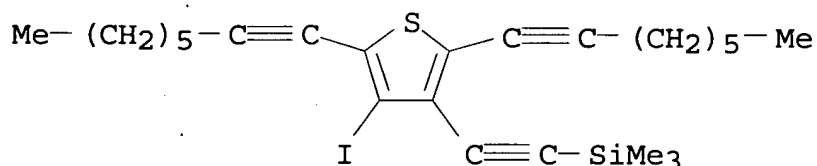
IT 252935-48-1P 252935-49-2P 252935-50-5P

252935-51-6P 252935-52-7P 252935-53-8P

(prepn. of tris(dialkynylthieno)cyclotriynes with long-chain alkyl substituents)

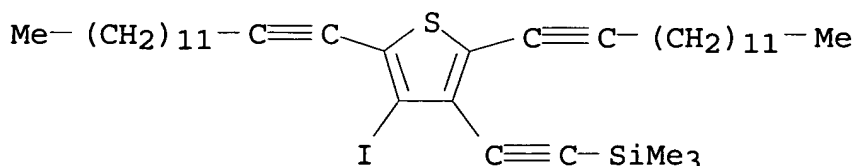
RN 252935-48-1 HCA

CN Silane, [(4-iodo-2,5-di-1-octynyl-3-thienyl)ethynyl]trimethyl- (9CI)
(CA INDEX NAME)



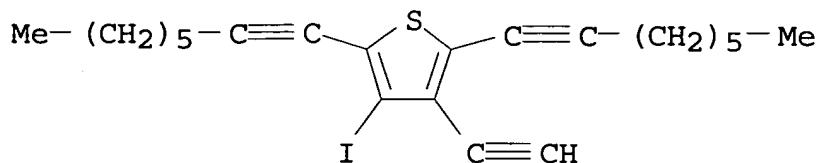
RN 252935-49-2 HCA

CN Silane, [(4-iodo-2,5-di-1-tetradecynyl-3-thienyl)ethynyl]trimethyl- (9CI)
(CA INDEX NAME)



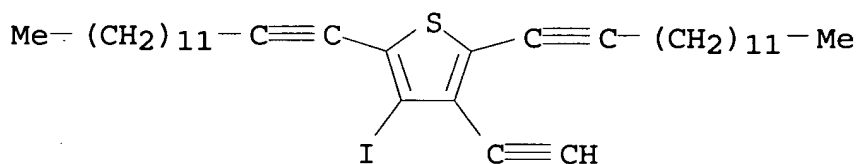
RN 252935-50-5 HCA

CN Thiophene, 3-ethynyl-4-iodo-2,5-di-1-octynyl- (9CI) (CA INDEX NAME)



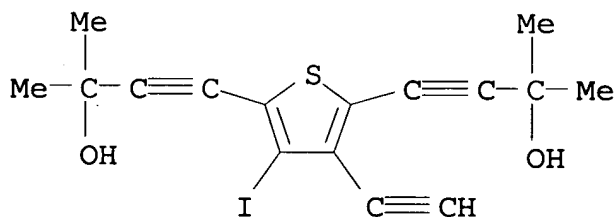
RN 252935-51-6 HCA

CN Thiophene, 3-ethynyl-4-iodo-2,5-di-1-tetradecynyl- (9CI) (CA INDEX NAME)



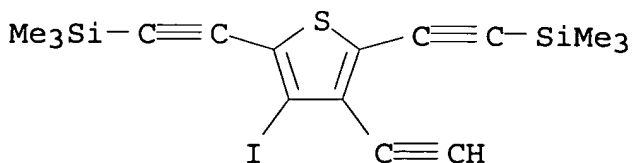
RN 252935-52-7 HCA

CN 3-Butyn-2-ol, 4,4'-(3-ethynyl-4-iodo-2,5-thiophenediyl)bis[2-methyl- (9CI) (CA INDEX NAME)



RN 252935-53-8 HCA

CN Silane, [(3-ethynyl-4-iodo-2,5-thiophenediyl)di-2,1-ethynediyl]bis[trimethyl- (9CI) (CA INDEX NAME)



CC 29-13 (Organometallic and Organometalloidal Compounds)
Section cross-reference(s): 25, 27, 28, 75

IT **Liquid crystals**

(attempted prepn. of discotic mesogens based on cyclotriyne core with alkyl side chain substituents)

IT 19259-11-1P, Tetraiodothiophene 113705-22-9P 252935-45-8P
252935-46-9P 252935-47-0P 252935-48-1P
252935-49-2P 252935-50-5P 252935-51-6P
252935-52-7P 252935-53-8P

(prepn. of tris(dialkynylthieno)cyclotriynes with long-chain alkyl substituents)

L40 ANSWER 14 OF 18 HCA COPYRIGHT 2005 ACS on STN

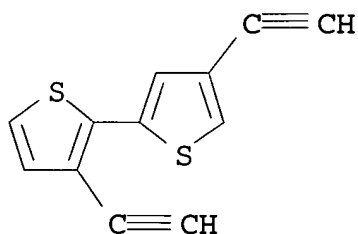
131:200453 Density functional theory investigation of substituent effects on building blocks of conducting polymers. Salzner, U. (Department of Chemistry, Bilkent University, Ankara, 06533, Turk.). Synthetic Metals, 101(1-3), 482-483 (English) 1999. CODEN: SYMEDZ. ISSN: 0379-6779. Publisher: Elsevier Science S.A..

AB Substituted heterocyclic dimers were calcd. by using d. functional theory (DFT) and analyzed with the natural bond orbital method (NBO). Substitution in 3- and 4-positions leads to parallel shifting of HOMO and LUMO but does not reduce energy gaps. For bridged dimers, HOMO-LUMO gaps correlate with .pi.-electron densities in the carbon backbone and energy gap redns. correlate with the strength of .pi.-.pi.* interactions from the backbone to the bridging group. Alternating donor-acceptor groups do not reduce energy gaps and lead to systems with av. HOMO and LUMO levels compared to the parent mols.

IT 220726-28-3
(substituent effects on building blocks of conducting polymers calcd. by d. functional theory)

RN 220726-28-3 HCA

CN 2,2'-Bithiophene, 3,4'-diethynyl- (9CI) (CA INDEX NAME)



CC 36-5 (Physical Properties of Synthetic High Polymers)

IT Band gap

Conducting polymers

Density functional theory

HOMO (molecular orbital)

LUMO (molecular orbital)

(substituent effects on building blocks of conducting polymers calcd. by d. functional theory)

IT 25796-77-4 113386-74-6 138050-21-2 152368-89-3 220726-25-0,
[2,2'-Bithiophene]-3,4'-diol 220726-26-1, [2,2'-Bithiophene]-3,4'-
diamine 220726-27-2, [2,2'-Bithiophene]-3,4'-dicarbonitrile
220726-28-3 241809-57-4 241809-58-5 241809-59-6
241809-60-9 241809-61-0 241809-62-1 241809-63-2 241809-64-3
241809-65-4 241809-66-5 241809-67-6 241809-68-7,
4H-Cyclopenta[2,1-b:3,4-b']difuran-4-one 241809-69-8 241809-70-1
241809-71-2 241809-72-3

(substituent effects on building blocks of conducting polymers
calcd. by d. functional theory)

L40 ANSWER 15 OF 18 HCA COPYRIGHT 2005 ACS on STN

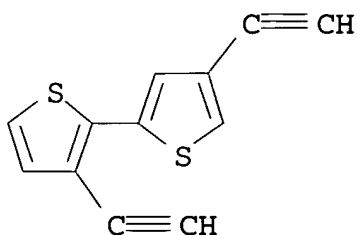
130:197214 Theoretical Analysis of Substituent Effects on Building
Blocks of Conducting Polymers: 3,4'-Substituted Bithiophenes.
Salzner, Ulrike; Kiziltepe, Tanyel (Department of Chemistry, Bilkent
University, Bilkent, 06533, Turk.). Journal of Organic Chemistry,
64(3), 764-769 (English) 1999. CODEN: JOCEAH. ISSN: 0022-3263.
Publisher: American Chemical Society.

AB To study substituent effects on energy levels and energy gaps
systematically, CH₃-, OH-, NH₂-, CN-, and CCH-substituted
bithiophenes were studied using d. functional theory and NBO
[natural bond orbital] anal. Total charges and .pi.-electron
densities were analyzed sep. to examine .pi.- and .sigma.-effects.
Second-order perturbation theory was used to quantify conjugation in
terms of orbital interactions. The NBO orbital energy was used to
study the effect of alternating donor-acceptor substitution.
Substituents in 3- and 4-positions shift HOMO and LUMO levels in
parallel and hardly influence HOMO-LUMO gaps. For level shifting,
the .pi.-donating and .pi.-accepting abilities are most important;
electronegativity mainly influences the .sigma.-orbitals and is less
crucial in detg. energy gaps. Alternating donor-acceptor
substitution leads to HOMO and LUMO energies that are av. between
those of the parent systems and has little effect on energy gaps.

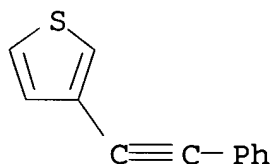
IT **220726-28-3**
(theor. anal. of substituent effects on 3,4'-substituted
bithiophene monomers and correlation with conducting polymers)

RN 220726-28-3 HCA

CN 2,2'-Bithiophene, 3,4'-diethynyl- (9CI) (CA INDEX NAME)



- CC 36-5 (Physical Properties of Synthetic High Polymers)
Section cross-reference(s): 76
- IT **Conducting polymers**
Density functional theory
Electronegativity
HOMO (molecular orbital)
LUMO (molecular orbital)
Natural bond orbital
(theor. anal. of substituent effects on 3,4'-substituted bithiophene monomers and correlation with conducting polymers)
- IT 56902-08-0, Bithiophene 113386-74-6, 3,4'-Dimethyl-2,2'-bithiophene 220726-25-0, 3,4'-Dihydroxy-2,2'-bithiophene 220726-26-1, [2,2'-Bithiophene]-3,4'-diamine 220726-27-2, [2,2'-Bithiophene]-3,4'-dicarbonitrile 220726-28-3 220726-29-4
(theor. anal. of substituent effects on 3,4'-substituted bithiophene monomers and correlation with conducting polymers)
- L40 ANSWER 16 OF 18 HCA COPYRIGHT 2005 ACS on STN
128:230943 Synthesis and electronic properties of poly(2-phenylthieno[3,4-b]thiophene). Neef, C. J.; Ferraris, J. P. (Department of Chemistry, The University of Texas at Dallas, Richardson, TX, 75083-0688, USA). Polymer Preprints (American Chemical Society, Division of Polymer Chemistry), 39(1), 147-148 (English) 1998. CODEN: ACPPAY. ISSN: 0032-3934. Publisher: American Chemical Society, Division of Polymer Chemistry.
- AB The synthesis of 2-phenylthieno[3,4-b]thiophene was accomplished in two steps beginning with 3,4-dibromothiophene and phenylacetylene in an overall yield of 29%. Repetitive cyclic voltammetry scans on acetonitrile solns. of this monomer showed good polymn. growth and the corresponding conductive polymer was obtained. Cyclic voltammetry shows an oxidn. potential of 0.40 V and a redn. potential of -2.2 V vs. Ag/Ag ion. The band gap of the polymer was estd. from the onset of oxidn. and redn. to be about 1.1 to 1.2 eV.
- IT **131423-29-5P**, 3-(Phenylethynyl)thiophene
(prepn. and oxidn. potential and band gap of poly(phenylthienothiophene) conducting polymer)
- RN 131423-29-5 HCA
CN Thiophene, 3-(phenylethynyl)- (9CI) (CA INDEX NAME)



- CC 36-5 (Physical Properties of Synthetic High Polymers)

Section cross-reference(s): 35, 76

IT Band gap

Conducting polymers

Oxidation potential

Reduction potential

(prepn. and oxidn. potential and band gap of
poly(phenylthienothiophene) conducting polymer)

IT **131423-29-5P**, 3-(Phenylethynyl)thiophene
(prepn. and oxidn. potential and band gap of
poly(phenylthienothiophene) conducting polymer)

L40 ANSWER 17 OF 18 HCA COPYRIGHT 2005 ACS on STN

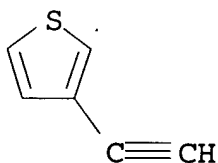
120:133616 Electronic structure of ethynylthiophenes. Novak, Igor; Ng, Siu Choon; Fang, Jiye; Mok, Chup Yew; Huang, Hsing Hua (Dep. Chem., Natl. Univ. Singapore, Singapore, 0511, Singapore). Journal of Physical Chemistry, 98(3), 748-51 (English) 1994. CODEN: JPCHAX. ISSN: 0022-3654.

AB He I and He II photoelectron spectra of all isomeric mono- and diethynylthiophenes were recorded. The electronic structure was analyzed and spectra were assigned on the basis of empirical considerations and semiempirical MO calcns. The spectra indicate various interactions taking place between thiophene .pi. and ethynyl .pi. orbitals. The relationship between deduced electronic structure and formation of novel polymer materials is discussed.

IT **67237-53-0**, 3-Ethynylthiophene
(photoelectron spectrum and electronic structure of)

RN 67237-53-0 HCA

CN Thiophene, 3-ethynyl- (9CI) (CA INDEX NAME)

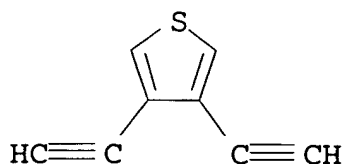


IT **138354-60-6P**, 3,4-Diethynylthiophene **153143-04-5P**,
2,3-Diethynylthiophene **153143-05-6P**, 2,4-
Diethynylthiophene

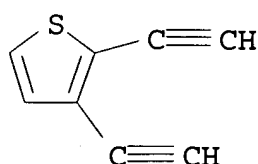
(prepn., photoelectron spectrum and electronic structure of)

RN 138354-60-6 HCA

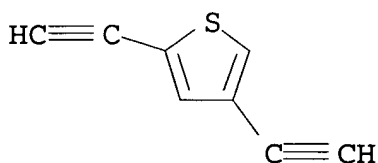
CN Thiophene, 3,4-diethynyl- (9CI) (CA INDEX NAME)



RN 153143-04-5 HCA
 CN Thiophene, 2,3-diethynyl- (9CI) (CA INDEX NAME)



RN 153143-05-6 HCA
 CN Thiophene, 2,4-diethynyl- (9CI) (CA INDEX NAME)



CC 22-9 (Physical Organic Chemistry)
 Section cross-reference(s): 35, 76
 IT Electronic structure
 Ionization potential and energy
 Molecular vibration
 Photoelectric emission
 (of ethynylthiophenes and diethynylthiophenes)
 IT 4298-52-6, 2-Ethynylthiophene 67237-53-0,
 3-Ethynylthiophene 79109-72-1, 2,5-Diethynylthiophene
 (photoelectron spectrum and electronic structure of)
 IT 138354-60-6P, 3,4-Diethynylthiophene 153143-04-5P,
 2,3-Diethynylthiophene 153143-05-6P, 2,4-Diethynylthiophene
 (prepn., photoelectron spectrum and electronic structure of)

L40 ANSWER 18 OF 18 HCA COPYRIGHT 2005 ACS on STN
 117:192371 Diacetylenes with formally conjugated side groups:
 precursors to liquid-crystalline polymers?. Sarkar, A.; Babu, K.
 Nagendra; Kamath, M. B.; Khandelwal, P. K.; Bhagwat, Lalita P.;
 Talwar, S. S. (Dep. Chem., Indian Inst. Technol., Bombay, 400 076,

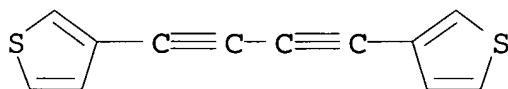
India). Front. Polym. Res., [Proc. Int. Conf.], 1st, 233-8.
 Editor(s): Prasad, Paras N.; Nigam, Jai Krishna. Plenum: New York,
 N. Y. (English) 1991. CODEN: 57ZRAI.

AB Liq.-cryst. diacetylenes having conjugated side groups had
 enthalpies of crystal-liq. crystal transition 4.13-8.5 kcal/mol.
 The diacetylenes polymd. upon heating and gave polymers that were
 not liq.-cryst. The heat of polymn. was 35-45 kcal/mol.

IT 81294-14-6 144091-95-2
 (liq.-cryst., thermal polymn. of, heat of)

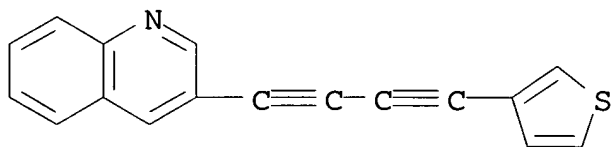
RN 81294-14-6 HCA

CN Thiophene, 3,3'-(1,3-butadiyne-1,4-diyl)bis- (9CI) (CA INDEX NAME)



RN 144091-95-2 HCA

CN Quinoline, 3-[4-(3-thienyl)-1,3-butadiynyl]- (9CI) (CA INDEX NAME)



CC 35-2 (Chemistry of Synthetic High Polymers)

IT **Liquid crystals**

(diacetylenes having conjugated side groups, thermal polymn. of,
 heat of)

IT 16900-51-9 20199-30-8 29768-12-5 81294-14-6
 104225-63-0 128295-74-9 144091-93-0 144091-94-1
 144091-95-2 144091-96-3 144091-97-4
 (liq.-cryst., thermal polymn. of, heat of)

=> d 141 1-30 ti

L41 ANSWER 1 OF 30 HCA COPYRIGHT 2005 ACS on STN

TI Discovery of novel conformationally constrained tropane-based biaryl
 and arylacetylene ligands as potent and selective norepinephrine
 transporter inhibitors and potential antidepressants

L41 ANSWER 2 OF 30 HCA COPYRIGHT 2005 ACS on STN

TI Process for preparing 3-acetylthiophene

L41 ANSWER 3 OF 30 HCA COPYRIGHT 2005 ACS on STN

- TI Highly efficient one-pot synthesis of N-sulfonylamidines by Cu-catalyzed three-component coupling of sulfonyl azide, alkyne, and amine
- L41 ANSWER 4 OF 30 HCA COPYRIGHT 2005 ACS on STN
- TI Crystal structure of methionine aminopeptidase from *Staphylococcus aureus* and *Streptococcus pneumoniae*, and use of structural data in drug discovery
- L41 ANSWER 5 OF 30 HCA COPYRIGHT 2005 ACS on STN
- TI Preparation of novel cyclosporins
- L41 ANSWER 6 OF 30 HCA COPYRIGHT 2005 ACS on STN
- TI Preparation, methylation, and coupling reaction of 1,2-dithienyl-3,4-bis[(2,4,6-tri-*t*-butylphenyl)phosphinidene]cyclobutenes
- L41 ANSWER 7 OF 30 HCA COPYRIGHT 2005 ACS on STN
- TI Novel 3-phenylprop-2-ynylamines as inhibitors of mammalian squalene epoxidase
- L41 ANSWER 8 OF 30 HCA COPYRIGHT 2005 ACS on STN
- TI Asymmetric synthesis of secondary propargyl alcohols
- L41 ANSWER 9 OF 30 HCA COPYRIGHT 2005 ACS on STN
- TI Acetylenic bond reduction anchored on $(\text{CO})_6\text{Fe}_2(\mu\text{-Se}_2)$: synthesis and characterization of $[(\text{CO})_6\text{Fe}_2\{\mu\text{-SeC(H):C(R)Se}\}]$ and $[(\text{CO})_6\text{Fe}_2\text{Se}_2]_2\{\mu\text{-C(H)=CR}\}]$ ($\text{R} = 3\text{-Th}, 2\text{-Th}; \text{Th} = \text{C}_4\text{H}_3\text{S}$)
- L41 ANSWER 10 OF 30 HCA COPYRIGHT 2005 ACS on STN
- TI Heteroaryl functionalized diacetylenes: preparation and solid-state reactivity
- L41 ANSWER 11 OF 30 HCA COPYRIGHT 2005 ACS on STN
- TI 3,4-Thienylene-ethynylene oligomers
- L41 ANSWER 12 OF 30 HCA COPYRIGHT 2005 ACS on STN
- TI Synthesis and electronic structure of 1,2-heteroarylethynes: potential monomers for low bandgap conductive polymers
- L41 ANSWER 13 OF 30 HCA COPYRIGHT 2005 ACS on STN
- TI An improved procedure for the preparation of aryl- and heteroarylacetylenes
- L41 ANSWER 14 OF 30 HCA COPYRIGHT 2005 ACS on STN
- TI Preparation and Structural Characterization of a Platinum Catecholate Complex Containing Two 3-Ethynylthiophene Groups

- L41 ANSWER 15 OF 30 HCA COPYRIGHT 2005 ACS on STN
 TI Routes towards three-dimensional fully conjugated conducting polymers: 1. Preparation of the kit of monomers
- L41 ANSWER 16 OF 30 HCA COPYRIGHT 2005 ACS on STN
 TI Flash vacuum pyrolysis of stabilized phosphorus ylides. Part 2. Two-step conversion of acid chlorides into acetylenic esters and terminal alkynes
- L41 ANSWER 17 OF 30 HCA COPYRIGHT 2005 ACS on STN
 TI Synthesis and characterization of trithienocyclotriyne (TTC) and its tetracobalt complex. The first example of a dehydroannulene containing thiophene rings
- L41 ANSWER 18 OF 30 HCA COPYRIGHT 2005 ACS on STN
 TI Oxyalkynes and their uses as inflammation inhibitors or antiasthmatics
- L41 ANSWER 19 OF 30 HCA COPYRIGHT 2005 ACS on STN
 TI Preparation of N-(propynylbenzyl)-N-hydroxyl-N-acylamines as 5- and 12-lipoxygenase inhibitors
- L41 ANSWER 20 OF 30 HCA COPYRIGHT 2005 ACS on STN
 TI A convenient method for the preparation of thienylacetylenes
- L41 ANSWER 21 OF 30 HCA COPYRIGHT 2005 ACS on STN
 TI Synthesis of a trithienocyclotriyne
- L41 ANSWER 22 OF 30 HCA COPYRIGHT 2005 ACS on STN
 TI Convenient two-step conversion of acid chlorides to terminal alkynes
- L41 ANSWER 23 OF 30 HCA COPYRIGHT 2005 ACS on STN
 TI Magnetic powder with improved dispersibility
- L41 ANSWER 24 OF 30 HCA COPYRIGHT 2005 ACS on STN
 TI The synthesis of 2,2':5',3"-terthiophene
- L41 ANSWER 25 OF 30 HCA COPYRIGHT 2005 ACS on STN
 TI Synthesis of 3,2':5',3"-terthiophene and other terthiophenes by the thiophenecarboxaldehyde .fwdarw. ethynylthiophene .fwdarw. dithienylbutadiyne route
- L41 ANSWER 26 OF 30 HCA COPYRIGHT 2005 ACS on STN
 TI General and simple syntheses of aryl- and heteroarylacetylenes
- L41 ANSWER 27 OF 30 HCA COPYRIGHT 2005 ACS on STN
 TI Chemistry of heterocyclics. XXV. Investigations on diacetylenes and diacetylenic glycols in the thiophene series

L41 ANSWER 28 OF 30 HCA COPYRIGHT 2005 ACS on STN
 TI Chemistry of heterocyclics. XXIV. Preparation of thienylacetylenes

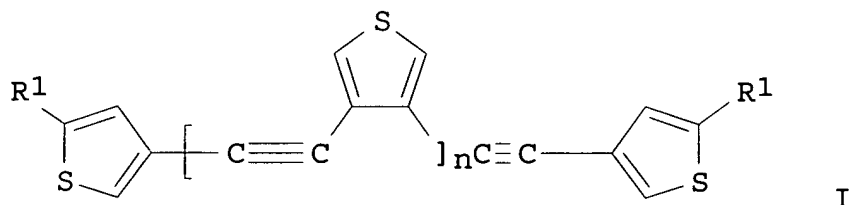
L41 ANSWER 29 OF 30 HCA COPYRIGHT 2005 ACS on STN
 TI Synthesis of .beta.-thienylacetylene

L41 ANSWER 30 OF 30 HCA COPYRIGHT 2005 ACS on STN
 TI Thienyl acetylenes

=> d l41 11,12,15 cbib abs hitstr hitrn

L41 ANSWER 11 OF 30 HCA COPYRIGHT 2005 ACS on STN
 127:331344 3,4-Thienylene-ethynylene oligomers. Aso, Yoshio;
 Nishiguchi, Shoji; Jigami, Tetsuya; Otsubo, Tetsuo; Ogura, Fumio
 (Dep. Applied Chem., Fac. Eng., Hiroshima Univ., Higashi-Hiroshima,
 739, Japan). Phosphorus, Sulfur and Silicon and the Related
 Elements, 120 & 121, 417-418 (English) 1997. CODEN: PSSLEC. ISSN:
 1042-6507. Publisher: Gordon & Breach.

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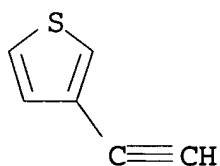


AB Several well-defined 3,4-thienylene-ethynylene oligomers (I) ($R_1 =$
 H, $n = 1, 3, 5, 7$) with different chain lengths have been
 synthesized and characterized. X-ray crystallog. analyses proved
 their unique, totally helical conformations.

IT 67237-53-0, 3-Ethynylthiophene
 (synthesis and conformation of thiophene-ethynylene oligomers)

RN 67237-53-0 HCA

CN Thiophene, 3-ethynyl- (9CI) (CA INDEX NAME)



IT 67237-53-0, 3-Ethynylthiophene
(synthesis and conformation of thiophene-ethynylene oligomers)

L41 ANSWER 12 OF 30 HCA COPYRIGHT 2005 ACS on STN

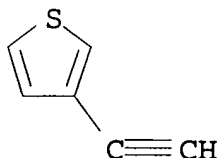
127:331111 Synthesis and electronic structure of 1,2-heteroarylethynes: potential monomers for low bandgap conductive polymers. Ng, S. C.; Novak, I.; Wang, L.; Huang, H. H.; Huang, W. (Department of Chemistry, National University of Singapore, Singapore, 119260, Singapore). Tetrahedron, 53(39), 13339-13350 (English) 1997. CODEN: TETRAB. ISSN: 0040-4020. Publisher: Elsevier.

AB A series of 1,2-heteroarylethynes which are potential monomers to low bandgap materials were synthesized and their He I photoelectron spectra measured and assigned with the aid of empirical arguments and semi-empirical MO calcns. The electronic structure anal. reveals that C.tplbond.C bond is an efficient relay of .pi.-electrons and that it supports inter-ring conjugation. The efficiency depends on the nature of ring heteroatom, but not on its position within the ring. The importance of C.tplbond.C bond relay is discussed in the broader context of conjugated polymer applications.

IT 67237-53-0, 3-Ethynylthiophene
(prepn. and photoelectron spectra of 1,2-heteroarylethynes)

RN 67237-53-0 HCA

CN Thiophene, 3-ethynyl- (9CI) (CA INDEX NAME)



IT 67237-53-0, 3-Ethynylthiophene
(prepn. and photoelectron spectra of 1,2-heteroarylethynes)

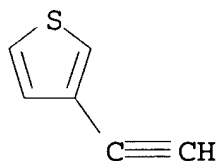
L41 ANSWER 15 OF 30 HCA COPYRIGHT 2005 ACS on STN

122:133929 Routes towards three-dimensional fully conjugated conducting polymers: 1. Preparation of the kit of monomers. Rebourt, Eymard; Pepin-Donat, Brigitte; Dinh, Emmanuel (Departement de Recherche Fondamentale sur la Matiere Condensee, CEA, Grenoble, 38054, Fr.). Polymer, 36(2), 399-412 (English) 1995. CODEN: POLMAG. ISSN: 0032-3861. Publisher: Elsevier.

AB Several trithienylbenzenes were prepd. and characterized. These compds. are used as reticulation points in poly(3-n-octylthiophene). It was necessary to study the reactivity of the reticulation points with regard to 3-n-octylthiophene. That is the reason why we have prepd. copolymers starting from very high percentages of deuterated reticulation points (>20%) and monitored their reactivities

following the evolution of the :C-D band in the IR spectra of the copolymers. The copolymers thus obtained contain from 10% to 30% of reticulation points. They swell in apolar solvents whereas the poly(reticulation point) (100% of reticulation points) does not swell. A low molar doping level ($\text{FeCl}_3 \cdot 6\text{H}_2\text{O}$, <9%) leads to a non-negligible cond. (0.1 to 0.2 S cm^{-1}) of these copolymers. In the same conditions, the poly(reticulation point) cannot be doped and thus remains insulating.

IT 67237-53-0P, 3-Ethynylthiophene
 (prepn. and characterization of)
 RN 67237-53-0 HCA
 CN Thiophene, 3-ethynyl- (9CI) (CA INDEX NAME)



IT 67237-53-0P, 3-Ethynylthiophene
 (prepn. and characterization of)